(19) World Intellectual Property Organization

International Bureau



(43) International Publication Date 5 February 2004 (05.02.2004)

PCT

(10) International Publication Number WO 2004/011640 A1

(51) International Patent Classification7: C07K 14/705, G01N 23/20, 33/573

C12N 9/48,

(21) International Application Number: PCT/JP2003/009523

(22) International Filing Date: 28 July 2003 (28.07.2003)

(25) Filing Language:

English

(26) Publication Language:

English

(30) Priority Data: 60/398,761

29 July 2002 (29.07.2002) US

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- (81) Designated States (national): AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW.
- (84) Designated States (regional): ARIPO patent (GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).

Published:

- with international search report
- before the expiration of the time limit for amending the claims and to be republished in the event of receipt of amendments

For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.

(54) Title: THREE-DIMENSIONAL STRUCTURE OF DIPEPTIDYL PEPTIDASE IV

(57) Abstract: A crystal of a dipeptidyl peptidase IV; a three-dimensional structural coordinate of the dipeptidyl peptidase IV; a method for obtaining a three-dimensional coordinate of a homolog protein of the dipeptidyl peptidase IV; a method for obtaining a three-dimensional structural coordinate of a crystal of a complex of the dipeptidyl peptidase IV and a effector of the dipeptidyl peptidase IV; a method for identifying pharmacophore of the effector of the dipeptidyl peptidase IV; a method for designing, identifying, evaluating or searching; the effector, and a program and a medium therefor for use of the three-dimensional structural coordinate.

WO 2004/011640 PCT/JP2003/009523

DESCRIPTION

THREE-DIMENSIONAL STRUCTURE OF DIPEPTIDYL PEPTIDASE IV

5 TECHNICAL FIELD

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The present invention relates to a crystal and a three-dimensional structural coordinate of a dipeptidyl peptidase IV, and an application thereof. More specifically, the present invention relates to a crystal and a threedimensional structural coordinate, a method for obtaining a three-dimensional structural coordinate of a homolog protein of a dipeptidyl peptidase IV, a method for obtaining a three-dimensional structural coordinate of a crystal of a complex of a dipeptidyl peptidase IV with an effector (e.g. inhibitor) of the dipeptidyl peptidase IV, a method for identifying a pharmacophore of an effector (e.g. inhibitor) of for the dipeptidyl peptidase IV, a method for identifying sites affecting the activity of the dipeptidyl peptidase IV, a method for designing, identifying, evaluating or searching an effector (e.g. inhibitor) of the dipeptidyl peptidase IV, and a program and a medium therefor for use of the three-dimensional structural coordinate, which are useful in the development of an effector (e.g. inhibitor) of the dipeptidyl peptidase IV, useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like; and an effector (e.g. inhibitor) of the dipeptidyl peptidase IV useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like.

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BACKGROUND ART

Dipeptidyl peptidase IV (hereinafter also referred to as DPPIV) is a cell membrane protein, which has been found in epithelial cell of small intestine, prostate gland, renal tubule, biliary tract and the like, activated T-cell, B-cell, NK-cell and the like. In the DPPIV, deduced active sites of DPPIV in the C-terminal side are located in extracellular portions and those in the N-terminal side are located in cytoplasm in a living body. Also, there has been suggested the relationship of the above-mentioned DPPIV with the activities of various cytokines such as interleukin-1β, interleukin-2, interleukin-3, interleukin-5, interleukin-6, interleukin-13, tumor necrosis factor-β and the like, and activities of various chemokines such as RANTES and the like in immune system [Rinsho Menneki (Clinical Immunology), 34, Revised and Enlarged Edition 19, 45-53, published by Kagaku Hyoronsha (2000), and the like].

As to the dipeptidyl peptidase IV, it has been shown that some amino acid residues can be involved in exhibition of the activity of the dipeptidyl peptidase IV by experiments such as biochemical experiments using inhibitors, experiments using mutants produced by site-directed mutagenesis [for example, see Misumi et al, *Biochim. Biophys. Acta*, 1131, 333-336 (1992), Ogata et al, *Biochemistry*, 31, 2582-2587 (1992) and the like].

However, it is difficult to know the three-dimensional structures for active sites from the information. Therefore, it is presently difficult to obtain the three-dimensional structural information for identifying, searching, evaluating or designing an interaction of the dipeptidyl peptidase IV and a compound that acts with the dipeptidyl peptidase IV on the level of three-dimensional structure and a

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novel compound capable of binding with and acting on the dipeptidyl peptidase IV.

DISCLOSURE OF INVENTION

A first object of the present invention is to provide a crystal of a dipeptidyl peptidase IV, which is useful for providing a three-dimensional structural coordinate as the information for designing, identifying, evaluating or searching an effector (e.g. inhibitor) of the dipeptidyl peptidase IV useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like. A second object of the present invention is to provide a three-dimensional structural coordinate of the crystal, which can provide the information for designing, identifying, evaluating or searching an effector (e.g. inhibitor) of the dipeptidyl peptidase IV useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like. A third object of the present invention is to provide a method for obtaining a three-dimensional structural coordinate of a homolog protein of the dipeptidyl peptidase IV, whereby refinement of a three-dimensional structural coordinate of a homolog protein of the dipeptidyl peptidase IV can be more readily performed. Furthermore, a fourth object of the present invention is to provide a method for obtaining a three-dimensional structural coordinate of a crystal of a complex of a dipeptidyl peptidase IV and an effector (e.g. inhibitor) of the dipeptidyl peptidase IV, which can provide the information for designing, identifying, evaluating or searching an

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effector (e.g. inhibitor) of the dipeptidyl peptidase IV which is useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like, and is excellent in avidity, biological activity, biological stability, absorbency to a living body, and which can favorably act on the dipeptidyl peptidase IV. A fifth object of the present invention is to provide a method for identifying a pharmacophore of the dipeptidyl peptidase IV and the effector (e.g. inhibitor) of the dipeptidyl peptidase IV, which can provide the information for designing, identifying, evaluating or searching an effector (e.g. inhibitor) of the dipeptidyl peptidase IV useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like, and is excellent in avidity, biological activity, biological stability, absorbency in a living body, and which can be favorably act on the dipeptidyl peptidase IV. A sixth object of the present invention is to provide a method for designing, identifying, evaluating or searching the effector (e.g. inhibitor) of the dipeptidyl peptidase IV, which can logically and conveniently provide the effector (e.g. inhibitor) of the dipeptidyl peptidase IV useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like, and is excellent in avidity, biological activity, biological stability, absorbency in a living body (in vivo), and which can be favorably act on the dipeptidyl peptidase IV. A seventh object of the present invention is to provide the effector (e.g. inhibitor) of the dipeptidyl peptidase IV useful as a modulatory agent of immune

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response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like. An eighth object of the present invention is to provide a program and a medium therefor, which can rapidly and conveniently perform design, identification, evaluation or search of the effector (e.g. inhibitor) of the dipeptidyl peptidase IV.

Concretely, the present invention relates to:

- [1] a crystal of a dipeptidyl peptidase IV, having characteristics sufficient to ensure a resolution capable of analyzing its three-dimensional structure up to the side chain level by X-ray crystallographic structural analysis;
- [2] the crystal according to the above [1], wherein the dipeptidyl peptidase IV is a soluble polypeptide comprising a region located at extramembrane in a full-length human dipeptidyl peptidase IV;
- [3] the crystal according to the above [1] or [2], wherein the dipeptidyl peptidase IV is a polypeptide having an amino acid sequence in which a transmembrane region is deleted from the amino acid sequence of SEQ ID NO: 2, and a tag peptide is optionally added to a C-terminal side or N-terminal side thereof;
- [4] the crystal according to any one of the above [1] to [3], wherein the crystal has a space group of $P2_12_12_1$, and a lattice constant of the unit cell of $|a| = 118.0 \pm 5.0$ Å, $|b| = 125.9 \pm 5.0$ Å, $|c| = 136.8 \pm 5.0$ Å, and $\alpha = \beta = \gamma = 90^{\circ}$, and is orthorhombic;
 - [5] the crystal according to any one of the above [1] to [4], wherein the crystal has the structural coordinate shown in Figure 4;
- 25 [6] the crystal according to any one of the above [1] to [4], wherein the

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crystal has a structural coordinate different from the structural coordinate as shown in Figure 4 via fluctuation of a protein;

- [7] a three-dimensional structural coordinate of a dipeptidyl peptidase IV, comprising the structural coordinate shown in Figure 4;
- 5 [8] a three-dimensional structural coordinate of a dipeptidyl peptidase IV, comprising a structural coordinate different from the structural coordinate as shown in Figure 4 via fluctuation of a protein;
 - [9] the three-dimensional structural coordinate according to the above [8], wherein the fluctuation of a protein is a state that is caused by molecular oscillation or temperature, and exhibits an activity for the dipeptidyl peptidase IV in a living body;
 - [10] the three-dimensional structural coordinate according to any one of the above [7] to [9], wherein the dipeptidyl peptidase IV is a soluble polypeptide comprising a region located at extramembrane in a full-length human dipeptidyl peptidase IV;
 - [11] the three-dimensional structural coordinate according to any one of the above [7] to [10], wherein the dipeptidyl peptidase IV is a polypeptide having an amino acid sequence in which a transmembrane region is deleted from the amino acid sequence of SEQ ID NO: 2, and a tag peptide is optionally added of to a C-terminal side or N-terminal side thereof:
 - [12] a three-dimensional structural coordinate of a region in a dipeptidyl peptidase IV, comprising the three-dimensional structural coordinate of the region selected from the group consisting of the following (a) to (d):
- (a) a region characterized by Ser 630, Asp 708 and His 740 in the amino acid sequence of SEQ ID NO: 2, and

all or a part of a group of the amino acid residues located in the adjacent area of each of the Ser 630, Asp 708 and His 740 in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural coordinate;

- 5 (b) a region characterized by Ser 630, Asp 708 and His 740 in the amino acid sequence of SEQ ID NO: 2, and all or a part of a group of the amino acid residues comprising amino acids capable of maintaining physicochemical characteristics physiologically equivalent to each of amino acids in the group of the amino acid residues located in the adjacent area of each of Ser 630, Asp 708 and His 740, in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural coordinate,
- (c) a region characterized by a group of amino acid residues comprising amino acids capable of maintaining physicochemical characteristics

 15 physiologically equivalent to each of Ser 630, Asp 708 and His 740 in the amino acid sequence of SEQ ID NO: 2, and all or a part of a group of the amino acid residues located in the adjacent area of said group of the amino acid residues in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural coordinate; and
 - (d) a region characterized by a group of amino acid residues comprising amino acids capable of maintaining physicochemical characteristics physiologically equivalent to each of Ser 630, Asp 708 and His 740 in the amino acid sequence of SEQ ID NO: 2, and all or a part of a group of amino acid residues comprising amino acids

capable of maintaining physicochemical characteristics physiologically equivalent to each of the amino acids in the group of the amino acid residues located in the adjacent area of said group of the amino acids, in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural coordinate,

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wherein the region in the dipeptidyl peptidase IV is a region involved in binding or interaction between the dipeptidyl peptidase IV and an effector of the dipeptidyl peptidase IV;

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[13] the three-dimensional coordinate according to the above [12], wherein the physicochemical characteristic is selected from the group consisting of features in shape of a three-dimensional structure, hydrophobicity, electric charge and pK;

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[14] a method for obtaining a three-dimensional coordinate of a homolog protein of a dipeptidyl peptidase IV, characterized in refining an electron density map of the homolog protein of the dipeptidyl peptidase IV comprising the amino acid sequence of SEQ ID NO: 2, based on all and/or a part of the three-dimensional coordinate of any one of the above [7] to [13], to give a three-dimensional structural coordinate;

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[15] a method for obtaining a three-dimensional structural coordinate of a crystal of a complex of a dipeptidyl peptidase IV and an effector of the dipeptidyl peptidase IV characterized in using all and/or a part of the three-dimensional structural coordinate of any one of the above [7] to [13], to give a three-dimensional structural coordinate;

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[16] a method for identifying pharmacophore of an effector of the dipeptidyl peptidase IV, characterized in identifying the pharmacophore based on all and/or

a part of the three-dimensional structural coordinate of any one of the above [7] to [13], and the steric conformation of the effector of the dipeptidyl peptidase IV; [17] a method for designing, identifying, evaluating or searching an effector of a dipeptidyl peptidase IV, characterized in designing, identifying, evaluating or searching a compound capable of acting on the dipeptidyl peptidase IV, based on all and/or a part of the three-dimensional structural coordinate of any one of the above [7] to [13];

- [18] the method according to the above [17], wherein the method for designing, identifying, evaluating or searching an effector comprises the steps of:
- (i) identifying a region to be targeted for binding or interaction with the effector in a dipeptidyl peptidase IV, based on all and/or a part of the three-dimensional structural coordinate according to any one of the above [7] to [13] and the steric conformation of the effector of the dipeptidyl peptidase IV;
- 15 (ii) identifying atoms or atomic groups capable of generating in the above region at least one intermolecular interaction selected from the group consisting of covalent bond, ionic interaction, ion-dipole interaction, dipole-dipole interaction, hydrogen bonding, van der Waals force, electrostatic interaction and hydrophobic interaction, with the atoms or atomic groups existing in a candidate compound; and
 - (iii) designing a compound based on the information of the above step (i) and/or (ii);
 - [19] the method according to the above [18], wherein the method further comprises the steps of:
- detecting an interaction between the dipeptidyl peptidase IV and the

designed, identified, evaluated or searched candidate compound,
wherein when an interaction is detected, the candidate compound is identified as
a compound capable of binding to the dipeptidyl peptidase IV, based on a degree
of the interaction as an index;

5 [20] the method according to the above [18] or [19], wherein the method further comprises the steps of:

contacting the dipeptidyl peptidase IV with the designed, identified, evaluated or searched candidate compound and measuring the activity of the dipeptidyl peptidase IV,

- wherein when an activity increases or decreases, the designed, identified, evaluated or searched candidate compound is identified as a compound having enhancing action or inhibitory action on the activity of the dipeptidyl peptidase IV, based on a degree of the increase or decrease as an index;
 - [21] an effector of the dipeptidyl peptidase IV obtainable by the method of any one of the above [17] to [20];
 - [22] a program and a medium therefor for use of the three-dimensional structural coordinate of any one of the above [7] to [13], wherein all and/or a part of the three-dimensional structural coordinate of any one of the above [7] to [13] is recorded;
- [23] the program and the medium according to the above [22], comprising a means for identifying, searching, evaluating or designing a compound capable of binding to the dipeptidyl peptidase IV or a compound having an enhancing action or inhibitory action on the activity for the dipeptidyl peptidase IV; and [24] the program and the medium according to the above [23], further comprising a means for displaying a three-dimensional graphic display of a

molecule.

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BRIEF DESCRIPTION OF THE DRAWINGS

Figure 1 is a photomicrograph of a crystal of a dipeptidyl peptidase IV, wherein the field of view is 4000 $\mu m \times 3000 \ \mu m$.

Figure 2 is a photograph for X-ray diffraction pattern of a crystal of dipeptidyl peptidase IV.

Figure 3 is a photograph showing a three-dimensional structure of a crystal of a dipeptidyl peptidase IV displayed by the program QUANTA (Accelrys, Inc.).

Figure 4 is a drawing showing a three-dimensional coordinate of a crystal of a dipeptidyl peptidase IV.

BEST MODE FOR CARRYING OUT THE INVENTION

In the present specification, amino acid residues are expressed by using 15 the following abbreviations, which have been adopted by the IUPAC-IUB Commission on Biochemical Nomenclature (CBN). Also, unless explicitly otherwise indicated, the amino acid sequences of peptides and proteins are identified from N-terminal to C-terminal, left terminal to right terminal, the N-terminal being identified as a first residue. Ala: alanine residue; Asp: aspartate residue; Glu: glutamate residue; Phe: phenylalanine residue; Gly: glycine residue; His: histidine residue; Ile: isoleucine residue; Lys: lysine residue; Leu: leucine residue; Met: methionine residue; Asn: asparagine residue; Pro: proline residue; Gln: glutamine residue; Arg: arginine residue; Ser: serine residue; Thr: threonine residue; Val: valine residue; Trp: tryptophane residue;

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Tyr: tyrosine residue; Cys: cysteine residue.

The crystal of the present invention is a crystal of a dipeptidyl peptidase IV, having a characteristic sufficient to ensure a resolution capable of analyzing its three-dimensional structure up to the side chain level by X-ray crystallographic structural analysis.

The "characteristic sufficient to ensure a resolution capable of analyzing three-dimensional structure up to the side chain level" is, for example,

- (1) being in a state that a molecule in a unit cell of a crystal has repeats with high regularity, namely, providing diffraction at high resolution;
- 10 (2) having suitable form and size; it is desired that for example, a crystal has at least one side grown to about 0.2 to about 0.5 mm, preferably a cubic crystal having three sides that have similarly grown, or a needle-shaped crystal having a width or thickness of about 0.2 mm or more;
 - (3) having chemical stability, dynamic stability and physical stability; and the like. In a case of the dipeptidyl peptidase IV, which is a polypeptide having a relatively large molecular weight, the term means characteristics sufficient to ensure a resolution of 3Å or less, preferably 2.8Å or less, more preferably 2.6Å or less.

The dipeptidyl peptidase IV used for the preparation of the crystal of the present invention may have a high purity sufficient for forming the crystal. In the present invention, the dipeptidyl peptidase IV used for the preparation of the crystal includes a soluble polypeptide consisting of a region located at extramembrane in a full-length human dipeptidyl peptidase IV, for example, a polypeptide in which a transmembrane region in the N-terminal side [namely the region including the transmembrane sites (the region containing at least the

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amino acid nos: 1-28 of SEQ ID NO: 2, preferably the region of the amino acid nos: 1-32)] is deleted from the amino acid sequence of a full-length human dipeptidyl peptidase IV of SEQ ID NO: 2, and a tag peptide is optionally added to a C-terminal side or N-terminal side of the amino acid sequence. Concrete examples include (I) a polypeptide in which a transmembrane region in the N-terminal side is deleted from the amino acid sequence of a full-length human dipeptidyl peptidase IV of SEQ ID NO: 2; and (II) a polypeptide in which a tag peptide is added to a C-terminal side or N-terminal side of the polypeptide of the above (I). In the polypeptide, since the transmembrane site is deleted therefrom, the polypeptide has excellent characteristics that anchoring to the membrane can be prevented, and the polypeptide is a secretory type and soluble. The tag peptide is not particularly limited. For example, a polyhistidine peptide (an oligopeptide consisting of 4 to 20 of histidine residues) or the like can be preferably used as the tag peptide.

SEQ ID NO: 2 shows the amino acid sequence of a full-length dipeptidyl peptidase IV of human colon.

The full-length dipeptidyl peptidase IV means a polypeptide of a dipeptidyl peptidase IV containing a region comprising a transmembrane site in the N-terminal side. The full-length dipeptidyl peptidase IV includes a polypeptide comprising the amino acid sequence of SEQ ID NO: 2, without being limited thereto, and encompasses its naturally occurring variant, artificially modified variant, a homolog and an ortholog derived from heterogeneous organism, and the like.

Concretely, the full-length dipeptidyl peptidase IV, besides the polypeptide comprising the amino acid sequence of SEQ ID NO: 2, includes

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conservative substitution variants, naturally occurring allelic variants and the like. Also, the full-length dipeptidyl peptidase IV includes a polypeptide having at least one, namely one or more conservative amino acid substitutions, as compared to the polypeptide comprising the amino acid sequence of SEQ ID NO: 2.

The polypeptide as described above may be a polypeptide having biological activities (namely dipeptidyl peptidase IV activity) similar to the polypeptide comprising the amino acid sequence of SEQ ID NO: 2. Concretely, there are included, for instance, a polypeptide having homology of usually about 80% or more, preferably about 90% or more, more preferably about 95% or more on the amino acid level, as compared to the full-length amino acid sequence of SEQ ID NO: 2; a polypeptide encoded by a nucleic acid capable of hybridizing with a nucleic acid consisting of the nucleotide sequence of SEQ ID NO: 1 (nucleotide sequence encoding a full-length dipeptidyl peptidase IV of human colon), under stringent conditions, or a complement thereof; and a polypeptide having deletion, substitution or addition of at least one amino acid, namely one or plural amino acids, preferably one or several amino acids in the amino acid sequence of SEQ ID NO: 2.

The number of deletion, substitution or addition of the amino acids may be to an extent that the biological activities [namely, dipeptidyl peptidase IV activity] are not lost, usually in the number of 1 to about 150, preferably 1 to about 75, more preferably 1 to about 40.

The crystallization is carried out by making a solution containing the desired protein (referred to as a protein solution) supersaturated state, based on the characteristics that the protein in solution state converts to non-soluble state

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and precipitates as a crystal when specific conditions are satisfied. Concretely, the protein can be precipitated by the following procedures 1. or 2.:

- 1. elevating the effective concentration of the protein:
- concretely, adding a precipitant such as a salt, polyethylene glycol or an organic solvent to a protein solution; reducing an amount of a solvent in the protein solution by evaporation or the like; or the like.
- 2. reducing a repulsive force, or increasing an attractive force between protein molecules:

concretely, adding an organic solvent such as an alcohol to a protein solution; changing a hydrogen ion concentration (pH) or temperature of the protein solution; or the like.

As the conditions for the crystallization, physical and chemical factors such as a hydrogen ion concentration (pH), a kind of buffer used and a concentration thereof, a kind of a precipitant added and a concentration thereof, protein concentration, salt concentration, temperature and the like can be involved. A method for controlling and investigating the factors includes batch methods, dialysis methods, vapor diffusion methods (hanging-drop method, sitting-drop method and the like) and the like, described, for instance, in Blundell, T. L. et al., *PROTEIN CRYSTALLOGRAPHY*, 59-82 (1976), published by Academic Press, or the like.

The method for crystallization includes the batch methods, dialysis methods, vapor diffusion methods and the like. By the above method, physical and chemical factors such as a hydrogen ion concentration (pH), a kind and a concentration of the buffer used, and a kind and a concentration of the precipitant used, and physical and chemical factors such as protein concentration, salt

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concentration and temperature can be also determined.

The hydrogen ion concentration (pH) can be adjusted with a buffer. It is desired that the buffer is a buffer having buffering action in a broad range of pH, and being capable of suppressing precipitation of a non-proteinous crystal between the co-existing ion in the solution used during crystallization and the precipitant or the like. The buffer includes Tris-hydrochloric acid buffer, phosphate buffer, cacodylate buffer, acetate buffer, citrate buffer, glycine buffer and the like.

The precipitant may be a substance capable of elevating an effective concentration of the protein or changing a hydrogen ion concentration (pH) of the protein solution. Generally, the precipitant includes salts such as ammonium sulfate, sodium sulfate, sodium phosphate, potassium phosphate, sodium citrate, ammonium citrate, sodium chloride, potassium chloride and ammonium chloride; polyethylene glycols having various average molecular weights of about 200, about 1000, about 2000, about 4000, about 6000, about 8000, about 20000 or the like; organic solvents such as 2-methyl-2,4-pentadiol, methanol, ethanol, isopropanol, butanol and acetone, and the like.

The protein concentration may be a concentration suitable for crystallization, and it is desired that the protein concentration is, for example, 1 to 50 mg/ml, preferably 5 to 20 mg/ml, more preferably 7 to 15 mg/ml.

It is desired that the temperature conditions are 3° to 25°C, preferably 12° to 22°C.

In the case where the crystallization is carried out by the batch method, the crystallization can be carried out by gradually adding a precipitant solution comprising a precipitant, buffer and the like, so as to form a layer on the top layer of the solution containing the dipeptidyl peptidase IV to give a mixture, or by gradually adding the solution comprising the dipeptidyl peptidase IV, so that the solution is an upper layer of the precipitant solution to give a mixture. Here, the mixture is allowed to stand in a tightly closed vessel.

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In the case where the crystallization is carried out by the dialysis method, the crystallization can be carried out by placing a solution comprising dipeptidyl peptidase IV in a size exclusion semi-permeable membrane, and placing a precipitant solution outside of the size exclusion semi-permeable membrane as a reservoir solution, thereby diffusing the reservoir solution to the solution comprising the dipeptidyl peptidase IV via the semi-permeable membrane.

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In the case where the crystallization is carried out by the hanging-drop method in the vapor diffusion method, the crystallization can be carried out by placing a mixed solution of a solution comprising the dipeptidyl peptidase IV and a precipitant solution in a closed vessel allowing to be hanged at a position above the upper space of a reservoir in which the precipitant solution is contained as a reservoir solution, wherein the vapor pressure of the reservoir solution in the reservoir is set to be lower than that of the mixed solution.

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In the case where the crystallization is carried out by the sitting-drop method in the vapor diffusion method, the crystallization can be carried out by placing a mixed solution comprising a solution comprising the dipeptidyl peptidase IV and a precipitant solution in a closed vessel at a position higher than the liquid surface of a reservoir in which the precipitant solution is contained as a reservoir solution, wherein the vapor pressure of the reservoir solution in the reservoir is set to be lower than that of the mixed solution.

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The crystallization can be carried out by the sitting-drop method from the

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viewpoint of obtaining excellent-quality and large crystal.

When the obtained crystal is a crystal insufficient to ensure the X-ray structural analysis, the crystal may be grown by a seeding method such as macroseeding method or micro-seeding method, using the obtained crystal as a seed crystal.

When the macro-seeding method is performed, it is desired that the seed crystal is a single crystal that can be isolated by procedures under microscope wherein the seed crystal has excellent external form (having excellent crystallinity). Also, it is desired that the seed crystal is washed with a drop of a solution obtained by diluting the precipitant, for example, by 0.5 to 1.0-fold. It is desired that the solution used for seeding of the seed crystal is a protein solution having a degree of supersaturation that the crystal grows but the crystal nuclei do not grow. On the other hand, when the micro-seeding method is performed, the form and size of the seed crystal are not particularly limited.

The sequence information for the dipeptidyl peptidase IV and cDNA encoding the dipeptidyl peptidase IV can be obtained from a known information source [GenBank/EMBL accession No: X60708; Misumi et al., *Biochim. Biophys. Acta*, 1131, 333-336, (1992); GenBank/EMBL accession No: M80536; Darmoul et al., *J. Biol. Chem.*, 267, 4824-4833, (1992)]. Therefore, the dipeptidyl peptidase IV or a soluble polypeptide thereof can be produced by using conventional means for gene engineering on the basis of the above sequence information.

The nucleic acid used for production of the dipeptidyl peptidase IV or a soluble polypeptide thereof may be any nucleic acid in which the encoded polypeptide exhibits a dipeptidyl peptidase IV activity. For example, a nucleic

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acid encoding a polypeptide consisting of the amino acid sequence in which a transmembrane region in the N-terminal side (a region containing at least the amino acid nos: 1-28, preferably the region of the amino acid nos: 1-32) is deleted from the full-length human dipeptidyl peptidase IV, and a tag peptide is optionally added to a C-terminal side or N-terminal side of the amino acid sequence.

The nucleic acid can be obtained by, for instance, obtaining a fragment comprising a nucleic acid encoding a full-length dipeptidyl peptidase IV or a part thereof by means of conventional DNA recombination technique, and appropriately arranging the obtained fragment.

SEQ ID NO: 1 shows a sequence of a nucleic acid encoding a full-length dipeptidyl peptidase IV of human colon.

The nucleic acid (DNA or RNA) encoding a full-length dipeptidyl peptidase IV includes, for instance, a nucleic acid comprising human nucleic acids comprising the nucleotide sequence of SEQ ID NO: 1 without being limited thereto, and includes its naturally occurring variant, artificially modified variant, a homolog or ortholog derived from heterogeneous organism.

In other words, besides the nucleic acid comprising the nucleotide sequence of SEQ ID NO: 1, the nucleic acid includes a nucleic acid capable of hybridizing with a nucleic acid comprising the nucleotide sequence of SEQ ID NO: 1 under stringent conditions, more preferably under high-stringent conditions), or a complement thereof (nucleic acid having a complementary sequence).

Concrete examples of the nucleic acid described above include, for instance, a nucleic acid having usually about 70% or more, preferably about 80%

or more, more preferably about 85% or more, still more preferably about 90% or more, still more preferably about 95% or more, homology to the nucleotide sequence of SEQ ID NO: 1, and it is preferable that the polypeptide encoded by the above nucleic acid has a dipeptidyl peptidase IV activity.

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The dipeptidyl peptidase IV activity can be measured by, for example, incubating in a 1.5 ml reaction mixture [composition: 1.5 mM substrate (Gly-Pro-paranitroanilide), 71 mM glycine-NaOH (pH 8.7)] at 37°C for 10 minutes, and determining the liberated paranitroanilide at the absorbance of 405 nm. One unit (1 U) of a dipeptidyl peptidase IV is defined as an amount of the enzyme required for liberating 1 µmol of paranitroanilide per 1 minute.

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In the present invention, the hybridization under stringent conditions can be carried out as normal stringent conditions by performing hybridization in a hybridization solution having a salt concentration of $6 \times SSC$ or an equivalent concentration thereto, under the temperature conditions of 50° to $70^{\circ}C$ for about 16 hours, and optionally performing pre-washing with a solution having a salt concentration of $6 \times SSC$ or an equivalent concentration thereto, and thereafter performing washing with a solution having a salt concentration of $1 \times SSC$ or an equivalent concentration thereof. Furthermore, as the conditions having still higher stringency (high-stringent conditions), the hybridization can be carried out by washing with a solution having a salt concentration of $0.1 \times SSC$ or an equivalent concentration thereto in the above method.

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The dipeptidyl peptidase IV used for the crystallization has purity that can form a crystal, and the purity can be confirmed by conventional means of confirming purity (for example, a method comprising electrophoresing a fraction by polyacrylamide gel electrophoresis, SDS-polyacrylamide gel electrophoresis

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or the like, and visualizing the fraction by silver staining, or the like).

The X-ray structural analysis data of the crystal can be obtained by subjecting the crystal of the present invention to an X-ray crystallographic structural analysis known to one of ordinary skill in the art [for example, see Blundell, T. L. et al., PROTEIN CRYSTALLOGRAPHY, 59-82 (1976), published by Academic Press, and the like], whereby a three-dimensional structural coordinate (a value showing the relationship of the spatial positions of each atom) and a three-dimensional structure model for the crystal can be obtained. Concretely, the three-dimensional structural coordinate of the dipeptidyl peptidase IV is obtained as an atomic coordinate by procedures comprising the steps of 1) irradiating the crystal of the present invention with a monochromatic X-ray to give an X-ray diffraction pattern, 2) obtaining X-ray diffraction intensity data from the X-ray diffraction pattern, 3) obtaining an electron density map by Fourier transform, and 4) allocating a polypeptide chain and side chain thereof on the electron density map based on the amino acid sequence of the polypeptide used for the crystal. Furthermore, the three-dimensional structure is clarified by molecule-modeling based on the three-dimensional structural coordinate. Therefore, the three-dimensional structural coordinate of the dipeptidyl peptidase IV obtained from the crystal of the present invention is also encompassed within the scope of the present invention.

The crystallographic parameters for the crystal are obtained from the X-ray diffraction intensity data of the crystal of the present invention. The crystal of the present invention is an orthorhombic crystal having a space group of $P2_12_12_1$, and a lattice constant of the unit cell of $|a| = 118.0 \pm 5.0$ Å, $|b| = 125.9 \pm 5.0$ Å, $|c| = 136.8 \pm 5.0$ Å, and $\alpha = \beta = \gamma = 90^\circ$. The crystal has a

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2.6Å resolution by X-ray crystallographic structural analysis, that is, the crystal has characteristics sufficient to ensure a resolution capable of analyzing up to the side chain level of the polypeptide.

It is a known fact to one of ordinary skill in the art that the same protein can be crystallized even under different conditions. Therefore, the present invention is not limited to only the conditions for crystallization, and the crystal that shows substantially the same crystallographic constants as those in the present invention are also encompassed within the scope of the present invention.

More concretely, the crystal of the dipeptidyl peptidase IV of the present invention has a structural coordinate as shown in Figure 4, or a structural coordinate different from the structural coordinate as shown in Figure 4 via fluctuation of a protein.

The crystal according to the present invention can also be used as a seed crystal for carrying out the crystallization of a polypeptide having a three-dimensional structure similar to that of the dipeptidyl peptidase IV used for, for example, carrying out the crystallization of the dipeptidyl peptidase IV, dipeptidyl peptidase IV-like proteins, homolog proteins and the like, which are derived from other organism species.

When the crystal of the present invention is irradiated with X-ray, a low-temperature measurement may be carried out, as described in Examples set forth below.

The X-ray structural analysis data are converted to a structure factor by evaluating the intensity of X-ray diffraction using MOSFILM Program Package (Version 6.1). Also, in order to obtain the information for the phase, multiple isomorphous replacement method or the like can be performed, for example, as

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described in Examples.

In the structural analysis, CCP4 (Collaborative Computational Project, Number 4, 1994, "The CCP4 Suite: Programs for Protein Crystallography," Acta Cryst. D50, 760-763) program or the like is used.

The three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention can be obtained, for example, as follows. Firstly, Fourier transform calculation is carried out using the differences between the diffraction intensity obtained from two kinds of isomorphous replacement crystals of mercury and the diffraction intensity obtained from native crystal, and investigating the large peaks provided by the heavy atoms (mercury) on the Patterson's diagram to determine the locations of each mercury atoms in the unit cell of the real space. The phase of the crystal structure factor for the native crystal is determined using the obtained location coordinate for the mercury atoms. Furthermore, refinement is performed using the crystal structure factor of the native crystal and two kinds of the crystal structure factors of the isomorphous replacement crystals of mercury, and the coordinate for each of the mercury atoms is more accurately determined. An electron density map for the crystal of the dipeptidyl peptidase IV in the real space is obtained using the phase of the crystal structure factor of the native crystal calculated from the refined mercury atoms coordinate. Furthermore, the electron density map is improved by performing smoothing and histogram matching for the electron density map of the solvent region, whereby an electron density map necessary and sufficient for building a molecular model can be obtained. Next, the sites corresponding to the amino acid residues of the dipeptidyl peptidase IV on the electron density map are identified using QUANTA (manufactured by Accelrys, Inc.) to build the

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molecular model to give a three-dimensional structural coordinate.

The three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention is shown in Figure 4. Figure 4 shows the obtained three-dimensional structural coordinates, according to the format of the Protein Data Bank, which is a notation generally used by one of ordinary skill in the art.

The three-dimensional structural coordinates shown in Figure 4 are those represented using the origin of the unit cell of the crystal as the origin of the three-dimensional space. The R factor that is considered as an index for the accuracy of the obtained molecular model is 24.89%, and the free R factor is 30.15%. In addition, the deviation in the interatomic bond distance from the ideal state of the three-dimensional structure (rms-deviation) and the deviation in the bond angle are 0.006Å and 1.305°, respectively. In the case, for instance, the three-dimensional structural coordinate of the present invention is used for the calculation by a computer, a novel structural coordinate obtained as a result of the operation for mathematical transfer, such as translation, rotation, or symmetry in the three-dimensional space without changing the relative configuration of the atoms, is also encompassed within the scope of the present invention. Furthermore, not only all of the three-dimensional structural coordinate of the present invention but also a part thereof are also encompassed within the scope of the present invention.

The three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention can be used, for example, as shown in Figure 3, for three-dimensional graphic displaying of the stereogram of the three-dimensional structure model, and for evaluation of the structure-activity relationship and the quantitative structure-activity relationship. Also, the structural features of the

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crystal of the present invention can be more concretely shown using the three-dimensional structural coordinate shown in Figure 4. The evaluation of the structure-activity relationship or quantitative structure-activity relationship by the three-dimensional structure model is also encompassed within the scope of the present invention.

According to the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, one of the characteristics of the dipeptidyl peptidase IV can be found in that the dipeptidyl peptidase IV has 273 molecules of bond water in an asymmetric unit and has 5 molecules of N-acetylglucosamine residues per 1 molecule of the dipeptidyl peptidase IV.

According to the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, the information for atoms or atomic groups of the side chain of the dipeptidyl peptidase IV, interacting with the atoms or atomic groups of a known effector of the dipeptidyl peptidase IV via an intermolecular interaction can be obtained.

Furthermore, according to the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, the information of regions in the dipeptidyl peptidase IV that are susceptible to binding or intermolecular interaction with the effector can be obtained.

In addition, according to the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, the information of the structure specific to the dipeptidyl peptidase IV, which is not found in proteins other than the dipeptidyl peptidase IV, can be obtained. Therefore, higher selectivity in the effector targeting a protein other than the dipeptidyl peptidase IV can be designed, when the effector also acts on the dipeptidyl peptidase IV.

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The intermolecular interaction includes covalent bond, ionic interaction, ion-dipole interaction, dipole-dipole interaction, hydrogen bonding, van der Waals force, electrostatic interaction, hydrophobic interaction and the like.

In the present specification, the atoms or atomic groups of the effector and atoms or atomic groups of the side chain of the dipeptidyl peptidase IV, which interact with each other via intermolecular interaction, are referred to as "pharmacophore."

Also, according to the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, the information for the structure specific for the dipeptidyl peptidase IV, which is not found in proteins other than the dipeptidyl peptidase IV, can be provided.

In addition, for example, when the measurement conditions are different in X-ray diffraction, or the three-dimensional structure of the complex in the solution is analyzed using multidimensional NMR, and the like, the three-dimensional structural coordinate may differ from that shown in Figure 4. The three-dimensional structural coordinate varies depending on the fluctuation of protein and the like, and is encompassed within the scope of the present invention.

In the present specification, the "fluctuation of protein" means a state that is caused by molecular oscillation, temperature and the like, and accompanied with the structural change that can exhibit an activity for the dipeptidyl peptidase IV in a living body.

Also, according to the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, one of the characteristics of the dipeptidyl peptidase IV resides in that the amino acid residues, Ser 630, Asp 708

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and His 740, which are involved in the activity deduced by experiments by using various active inhibitors of the dipeptidyl peptidase IV, exist in the adjacent area, even though the amino acid residues exist in distant locations on the primary sequence. Concretely, the distance between the $O_{\delta 2}$ atom of Asp 708 and the $N_{\delta 1}$ atom of His 740, and the distance between the $N_{\epsilon 2}$ atom of His 740 and the O_{γ} atom of Ser 630 are distances that can form hydrogen bonding.

Therefore, the present invention also includes a three-dimensional structural coordinate of the region in the dipeptidyl peptidase IV, which is involved in binding or interaction of the dipeptidyl peptidase IV with an effector thereof, including a three-dimensional structural coordinate of a region selected from the group consisting of the following (a) to (d):

- (a) a region characterized by Ser 630, Asp 708 and His 740 in the amino acid sequence of SEQ ID NO: 2, and all or a part of a group of amino acid residues located in the adjacent area of each of the Ser 630, Asp 708 and His 740 in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural coordinate;
- (b) a region characterized by Ser 630, Asp 708 and His 740 in the amino acid sequence of SEQ ID NO: 2, and
 20 all or a part of a group of amino acid residues comprising amino acids capable of maintaining physicochemical characteristics physiologically equivalent to each of amino acids of the group of amino acid residues located in the adjacent area of each of Ser 630, Asp 708 and His 740, in the structural coordinate shown in Figure 4 or the three-dimensional
 25 structure model defined by the structural coordinate.

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- (c) a region characterized by a group of amino acid residues comprising amino acids capable of maintaining physicochemical characteristics physiologically equivalent to each of Ser 630, Asp 708 and His 740 in the amino acid sequence of SEQ ID NO: 2, and
- all or a part of a group of amino acid residues located in the adjacent area of said group of the amino acid residue in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural coordinate; and
- (d) a region characterized by a group of amino acid residues comprising
 amino acids capable of maintaining physicochemical characteristics
 physiologically equivalent to each of Ser 630, Asp 708 and His 740 in the
 amino acid sequence of SEQ ID NO: 2, and

all or a part of a group of amino acid residues of a group of amino acid residues comprising amino acids capable of maintaining physicochemical characteristics physiologically equivalent to the each amino acid of the amino acid residues located in the adjacent area of said groups of the amino acids, in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural coordinate.

In the present specification, the "adjacent (area)" refers to an area involved in covalent bond, ionic interaction, ion-dipole interaction, dipole-dipole interaction, hydrogen bonding, van der Waals force, electrostatic interaction, hydrophobic interaction or the like with the amino acid residues, concretely, a region within 10Å, preferably within 8Å, more preferably within 5Å.

The physicochemical characteristic includes features in shape of the three-dimensional structure, hydrophobicity, electric charge, pK and the like.

The "amino acid capable of maintaining physicochemical characteristics physiologically equivalent" may be an amino acid analogue residue obtained by replacing a side chain of amino acid residues in the three-dimensional structural coordinate shown in Figure 4 with other side chain, for example, showing bioisosterism. Alternatively, the amino acid residue in the three-dimensional structural coordinate shown in Figure 4, may be replaced with another amino acid residue belonging to the same Group, in any of the following Groups I to VI:

I glycine, alanine;

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10 II valine, isoleucine, leucine;

III aspartic acid, glutamic acid, asparagine, glutamine;

IV serine, threonine;

V lysine, arginine;

VI phenylalanine, tyrosine.

According to the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, a three-dimensional structural coordinate of a polypeptide can be easily derived if an accurate amino acid sequence is determined, even when the polypeptide is a dipeptidyl peptidase IV or a dipeptidyl peptidase IV-like protein derived from other organism species, as long as the polypeptide is a polypeptide having high homology on the level of amino acid sequence with the dipeptidyl peptidase IV used for the preparation of the crystal of the present invention (for example, at least 20%, preferably 30% or more, more preferably 40% or more).

Furthermore, the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention can be used for X-ray crystallographic

structural analysis of the crystal and the like of other proteins having an amino acid sequence with significant homology with the dipeptidyl peptidase IV used for the preparation of the crystal of the present invention. Concretely, according to the molecular replacement method [for example, see Blundell, T. L. et al., PROTEIN CRYSTALLOGRAPHY, 446-464 (1976), published by Academic Press and the like], the three-dimensional structural coordinate thereof can be quickly and readily obtained from the structure factors obtained by the X-ray diffraction pattern of the crystal, without using multiple isomorphous replacement method, even for the determination of the structural coordinate of the above-mentioned crystal of which structural coordinate has not yet been known.

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In the present specification, the term "significant homology" is a case where there is identity of 20%, or more, preferably by 30% or more, between the amino acid sequences.

When the molecular replacement method is performed, for example, a program such as X-PLOR and CNX (both manufactured by Accelrys Inc.) or AMORE [one of the programs of CCP4 (Collaborative Computational Project, Number 4), *Acta Crystallogr.* **D50**, 670-673 (1994)] can be run by a computer on which the program can be executed. Here, whether or not the molecular replacement method is applicable can be determined by actually applying the molecular replacement method to the structure factors calculated from the X-ray diffraction pattern of the desired crystal and obtaining a significant solution.

In other words, the three-dimensional structural coordinate obtained by structural analysis by molecular replacement method is encompassed within the scope of the present invention as long as a significant solution is obtained. The present invention also encompasses a three-dimensional structural coordinate of

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a dipeptidyl peptidase IV, or a dipeptidyl peptidase IV-like protein, namely a homolog protein or the like of other organism species derived by the above method.

Therefore, according to the present invention, a method for obtaining a three-dimensional structural coordinate of a homolog protein of a dipeptidyl peptidase IV comprising the step of performing refinement of an electron density map of the homolog protein of the dipeptidyl peptidase IV comprising the amino acid sequence of SEQ ID NO: 2, based on the three-dimensional structural coordinate of the present invention, to give a three-dimensional structural coordinate is provided. Also, a method for obtaining a three-dimensional structural coordinate of a crystal of a complex of a dipeptidyl peptidase IV and an effector of the dipeptidyl peptidase IV, based on the three-dimensional structural coordinate of the present invention, is likewise provided.

According to the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, a method for identifying a region or site for a target for binding or interaction between the dipeptidyl peptidase IV and an effector of the dipeptidyl peptidase IV is provided, based on the analysis of the binding regions between the dipeptidyl peptidase IV and a known effector of the dipeptidyl peptidase IV such as an inhibitor, or based on the simulation of the interaction between the dipeptidyl peptidase IV and a known effector of the dipeptidyl peptidase IV.

Also, based on the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention and the steric conformation of the effector of the dipeptidyl peptidase IV, the pharmacophore of the effector of the dipeptidyl peptidase IV can be identified. A method for identifying the

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pharmacophore is also provided. The method is useful for designing an effector having excellent characteristics such as higher avidity, higher biological activity, higher biological stability, higher thermodynamic stability, higher absorbency to a living body, and lower toxicity.

Concretely, for example, the region or site for a target involved in binding or interaction of the dipeptidyl peptidase IV and an effector of the dipeptidyl peptidase IV, can be identified by:

- 1) obtaining a crystal of a complex of the dipeptidyl peptidase IV and a known effector of the dipeptidyl peptidase IV such as an inhibitor, and obtaining a three-dimensional structural coordinate of the crystal based on the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention and the steric conformation of the effector of the dipeptidyl peptidase IV, whereby obtaining the three-dimensional structural coordinate of a binding region of the dipeptidyl peptidase IV and the effector;
- 2) simulating an intermolecular interaction between the dipeptidyl peptidase IV and a known effector of the dipeptidyl peptidase IV based on the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention and the steric conformation of the effector of the dipeptidyl peptidase IV;

or the like.

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The crystal of the above-mentioned complex can be obtained by, for example, incubating the crystal of the present invention in a solution comprising the effector, forming a complex of the dipeptidyl peptidase IV and the effector, and crystallizing the obtained complex, and the like.

Also, when the three-dimensional structural coordinate of the crystal of

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the complex is obtained, the steric structure of the effector of the abovementioned complex can be readily obtained by calculating the differential Fourier diagram utilizing a three-dimensional structure model defined by the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, whereby specific interaction forms and interaction sites between the dipeptidyl peptidase IV and the effector can be readily clarified.

When the intermolecular interaction is simulated, for example, the space regions, residues and the like in which covalent bond, ionic interaction, ion-dipole interaction, dipole-dipole interaction, hydrogen bonding, van der Waals force, electrostatic interaction, hydrophobic interaction or the like can be simulated, based on the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention and the steric conformation of the effector of the dipeptidyl peptidase IV.

Furthermore, according to the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, the three-dimensional structural coordinate or the three-dimensional structure model based on the three-dimensional structural coordinate regarded as an active center of the dipeptidyl peptidase IV, sites indirectly acting on the active center and regions or sites involved in binding or interaction with the effector, or the like, is obtained, whereby a compound capable of specifically acting on the dipeptidyl peptidase IV can be designed, identified, evaluated or searched.

For example, in the structural coordinate of Figure 4 and the threedimensional structure model defined by the structural coordinate, a compound capable of modifying the activity of the dipeptidyl peptidase IV can be designed, identified, evaluated or searched, based on the regions characterized by Ser 630,

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Asp 708 and His 740, and all or a part of amino acid residues of the group of the amino acid residues located in the adjacent area of the Ser 630, Asp 708 and His 740.

Therefore, according to the present invention, a method for designing, identifying, evaluating or searching an effector of the dipeptidyl peptidase IV is provided.

One of the significant features of the method of the present invention for designing, identifying, evaluating or searching an effector resides in that the method comprises designing, identifying, evaluating or searching a compound capable of acting on the dipeptidyl peptidase IV, based on the three-dimensional structural coordinate of the present invention.

According to the method of the present invention for designing, identifying, evaluating or searching an effector, since the method is based on the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, the information for a structure specific to the dipeptidyl peptidase IV, which is not found in proteins other than the dipeptidyl peptidase IV can be obtained. Therefore, according to the method of the present invention for designing, identifying, evaluating or searching an effector, the method has an excellent effect that the selectivity of the effector of the dipeptidyl peptidase IV can be enhanced.

Also, according to the method of the present invention for designing, identifying, evaluating or searching an effector, since the method is based on the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, visual studies and/or energy calculation can be made according to the method by using a computer and the like. Therefore, there are

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exhibited some excellent effects that a compound having excellent characteristics such as having higher avidity, higher biological activity, higher biological stability, higher thermodynamic stability, higher absorbency in a living body, and lower toxicity, than those for a known inhibitor can be designed, identified, evaluated or searched, and that logical design can be performed in the three-dimensional space.

In the present specification, the "effector" includes a compound that inhibits or enhances the activity (i.e. inhibitor or activator), which may be natural compounds or synthetic compounds, or may be polymers or low-molecular weight compounds.

A concrete example of the method of the present invention for designing, identifying, evaluating or searching an effector includes a method comprising the steps of:

- (i) identifying a region to be targeted for binding or interaction with the effector in a dipeptidyl peptidase IV, based on all and/or a part of the three-dimensional structural coordinate of the present invention and the steric conformation of the effector of the dipeptidyl peptidase IV;
- (ii) identifying corresponding atoms or atomic groups capable of generating in the region at least one intermolecular interaction selected from the group consisting of covalent bond, ionic interaction, ion-dipole interaction, dipole-dipole interaction, hydrogen bonding, van der Waals force, electrostatic interaction and hydrophobic interaction, with the atoms or atomic groups existing in a candidate compound; and
- (iii) designing a compound based on the above information of the above step(i) and/or (ii).

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The three-dimensional structural coordinate used for designing, identifying, evaluating or searching a compound capable of binding to the dipeptidyl peptidase IV may be a coordinate fixed in the three-dimensional space, and the intensity of binding with the compound or the like can be calculated by carrying out translation or rotation in the three-dimensional space, and transfer to an extent that the chemical covalent bond would not be cleaved in the amino acid residues of the dipeptidyl peptidase IV.

In the above step (i), the "region to be targeted in the dipeptidyl peptidase IV" preferably includes an active center of the dipeptidyl peptidase IV, sites indirectly acting on the active center and the like. For example, there is included a region characterized by Ser 630, Asp 708 and His 740 and all or a part of a group of the amino acid residues located in the adjacent area of Ser 630, Asp 708 and His 740, and the like in the structural coordinate of Figure 4 and the three-dimensional structure model defined by the structural coordinate. The atoms or atomic groups that can be matched therewith are identified, based on the three-dimensional structural coordinate of an active center, sites indirectly acting on the active center and the like, whereby the candidate atoms or candidate atomic groups can be obtained.

In the above step (ii), for example, the atoms or atomic groups capable of associating via intermolecular interaction between the atoms or atomic groups in the region, concretely, the corresponding atoms or atomic groups capable of generating covalent bond, ionic interaction, ion-dipole interaction, dipole-dipole interaction, hydrogen bonding, van der Waals force, electrostatic interaction, hydrophobic interaction and the like, are searched and extracted, based on the information identified in the above step (i).

Next, in the above step (iii), the corresponding atoms or atomic groups searched in the above step (i) and/or (ii) are combined to design a compound.

Thereafter, if desired, whether or not the compound designed in the above step (iii) is matched via intermolecular interaction with the side chains and atoms or atomic groups in the dipeptidyl peptidase IV as defined by the three-dimensional structural coordinate of the present invention can be simulated.

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The compound designed, identified, evaluated or searched by the above steps (hereinafter also referred to as a candidate compound in the present specification) can be obtained by generally used chemical synthetic methods, depending on the compound.

In addition, in the method of the present invention for designing, identifying, evaluating or searching an effector, there can be carried out a step of detecting the interaction between the dipeptidyl peptidase IV and the candidate compound. When the interaction is detected, the interaction serves as an index showing that the above candidate compound is a compound capable of binding to the dipeptidyl peptidase IV.

The above interaction can be detected by, for example, plasmon resonance analysis apparatus, mass spectrometer, titration isothermal calorimetry, NMR and the like. For example, in the case of plasmon resonance analysis apparatus, when a sensorgram indicates the formation of a complex, by contacting the dipeptidyl peptidase IV-immobilized matrix with the candidate compound and performing analysis by optical detection (for example, photometer, polarization photometer and the like) and the like, it would be an index showing that the interaction between the candidate compound and the dipeptidyl peptidase IV is generated. For example, in the case of a mass spectrometer, when a spectrum

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indicates the formation of a complex, by contacting the dipeptidyl peptidase IVimmobilized matrix with the candidate compound and performing analysis with a mass spectrometer (matrix-assisted laser desorption/ionization-time of flight mass spectrometry: MALDI-TOF MS, electro spray-ionization mass spectrometer: ESI-MS and the like), it would be an index showing that the interaction between the candidate compound and the dipeptidyl peptidase IV is generated. For example, in the case of titration-thermal calorimetry interaction analysis, when the titration curve indicates the formation of a complex, by contacting a solution of the dipeptidyl peptidase IV with the candidate compound, and measuring the heat coming in and out of a thermal diode and the like, it would be an index showing that the interaction between the candidate compound and dipeptidyl peptidase IV is generated. For example, in the case of NMR, when a spectrum indicates the formation of a complex, by analyzing by NMR a solution prepared mixing the dipeptidyl peptidase IV and a candidate compound, it would be an index showing that the interaction between the candidate compound and the dipeptidyl peptidase IV is generated.

Furthermore, the method of the present invention for designing, identifying, evaluating or searching an effector may further comprise the steps of contacting the dipeptidyl peptidase IV with a candidate compound, and thereafter measuring the activity of the dipeptidyl peptidase IV. When the dipeptidyl peptidase IV activity increases or decreases, it would be an index showing that the candidate compound is a compound having enhancing action or inhibitory action on the activity of the dipeptidyl peptidase IV.

The dipeptidyl peptidase IV activity can be measured by, for example, incubating a 1.5 ml reaction mixture [composition: 1.5 mM substrate

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(Gly-Pro-paranitroanilide), 71 mM glycine-NaOH (pH 8.7)] at 37°C for 10 minutes in the presence of a candidate compound, and measuring the liberated paranitroanilide at the absorbance of 405 nm. During the measurement of the activity, the candidate compound may be evaluated by using a reaction system in which a suitable dilution series of the compound is added thereto.

The method of the present invention for designing, identifying, evaluating or searching the effector can be performed by, for example, sequentially selecting the interaction between the dipeptidyl peptidase IV and the compounds in a database in a computer to which the structures of plural of compounds had been inputted, or the interaction between the dipeptidyl peptidase IV and the designed compound, by visual methods (visual selection method) utilizing the database; and/or sequentially calculating the avidity with a computer, and searching a compound capable of stably interacting with the dipeptidyl peptidase IV from the database (computer-assisted avidity evaluation method) and the like, based on the three-dimensional structural coordinate of the present invention.

In the above visual selection method, the database of the structures of compounds may be a database in which the three-dimensional structural coordinates have been determined and inputted. Alternatively, in the case of a compound having a low molecular weight, the database may be a database in which the information for chemical covalent bond of a compound having a low molecular weight had been inputted, because the conformation can be relatively freely changed, and the three-dimensional structural coordinate of each conformation can be derived by calculation in a relatively short time.

Concretely, in the visual selection method, the expected complex between the dipeptidyl peptidase IV and a candidate compound or a part thereof is firstly

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displayed on a computer screen, based on the three-dimensional structural coordinate of the present invention. Next, the intermolecular interaction binding between a compound in the database and the binding regions of the dipeptidyl peptidase IV is simulated on the computer, taking chemical interaction into consideration. Also, the simulation of the chemical modification of the compound is performed on the computer, and the changes in the interaction caused as a result thereof are observed on the computer screen. During the simulation, the three-dimensional space can be more easily understood by displaying the three-dimensional structure of the protein on the computer screen so that the structure corresponds to Crystal Eye glasses supplied by Silicone Graphics; simultaneously displaying two screens in which each angle is adjusted for displaying the object, according to the visual fields of the right eye and left eye, which is so-called referred to as "stereovision" which is frequently used by one of ordinary skill in the art; or the like. In addition, the three-dimensional structure can be visually studied by methods other than the stereoscopic displaying of the three-dimensional structure.

The candidate compound capable of generating suitable interaction can be obtained by displaying on a computer a group of candidates with appropriate conformation and selecting an appropriate one therefrom; calculating a structure having a low energy state on a computer; or the like. Next, a derivative of a compound capable of generating more preferable binding with the dipeptidyl peptidase IV may be searched among the candidate compound.

More specifically, on the level of the three-dimensional structure, the followings may be taken into consideration:

25 a group likely to be charged negatively, such as carboxyl group, nitro

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group, or a halogen group in the compound interacts with an amino acid residue having a positive charge, such as lysine, arginine or histidine in the dipeptidyl peptidase IV;

- a group likely to be charged positively, such as amino group, imino group or guanidyl group in the compound interacts with an amino acid residue having negative charge, such as glutamic acid or aspartic acid in the dipeptidyl peptidase IV;
- a hydrophobic functional group such as an aliphatic group or an aromatic group in the compound interacts with a hydrophobic amino acid residue such as alanine, leucine, isoleucine, valine, proline, phenylalanine, tryptophane or methionine in the dipeptidyl peptidase IV;
 - a group involved in hydrogen bonding, such as hydroxyl group or amide group is allowed to form hydrogen bonding with a main chain or side chain portion;
- a group or an atom likely to be charged negatively, such as carboxyl group, nitro group or a halogen group in the compound interacts with a positively charged atom on a main chain or side chain portion;
 - a group or an atom likely to be charged positively, such as amino group, imino group or guanidyl group in the compound interacts with a negative charged atom on a main chain or a side chain portion;
 - the flexibility of the three-dimensional structure of the compound is lowered by, for instance, cyclizing the linear chain portion; or the like. For example, a derivative may be designed and synthesized so that the atoms having negative charge of the candidate compound are located in the adjacent region of the side chain of an amino acid residue having positive charge

such as lysine, arginine or histidine, in the amino acid residue of the dipeptidyl peptidase IV, and that an atom having positive charge of the candidate compound is located in the adjacent region of the side chain of the amino acid residue having negative charge such as glutamic acid or aspartic acid in the amino acid residue of the dipeptidyl peptidase IV. Also, a group suitable for forming a hydrophobic interaction may be introduced into the portion capable of forming a hydrophobic interaction between the compound and the dipeptidyl peptidase IV, to design and synthesize a derivative. In addition, a group suitable for forming hydrogen bonding may be introduced into the portion capable of forming hydrogen bonding between the compound and the dipeptidyl peptidase IV, to design and synthesize a derivative. In the above-mentioned designing, it is desirable that van der Waals interaction is as high as possible, and that steric hindrance does not occur between each of the atoms. Furthermore, it is desirable that new void portions are not produced by modification of the compound and that in regions already containing void portions, the void portions are filled as much as possible.

As described above, the design, identification, evaluation or searching of a final compound can be thus performed with visually comprehensively considering intermolecular interaction and other factors on a computer screen.

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In the computer-assisted avidity evaluation method, in order to determine the validity for the designing of a new compound, and to obtain a compound that can stably interact from the compounds in the database, a docking software (DOCK, GOLD, FlexX, Glide or the like) is used for evaluation of binding based on the energy by calculating a molecular force field between the compound and the dipeptidyl peptidase IV, evaluation of binding based on chemical

characteristics, evaluation of binding based on the Protein Data Bank (PDB), and the like. Further, in a model system consisting of the compound and the dipeptidyl peptidase IV, or in a model system further comprising solvent molecules and the like, it can be led to a compound that can stably interact by obtaining the index showing avidity, such as free energy of bonding, the ratio obtained from bond state number and non-bond state number, and the like by using molecular kinetic calculation or Monte Carlo calculation. The programs for calculation of molecular force field and molecular kinetic include AMBER, CHARMm, DISCOVER, PRESTO and the like, and the force field used includes AMBER, CHARMm, OPLS, MMCF, CVFF and the like. Furthermore, a program such as Ludi which automatically outputs the candidates for a candidate compound by providing a three-dimensional structural coordinate of the amino acid residues interacting in the dipeptidyl peptidase IV may be used.

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The visual selection method and computer-assisted avidity evaluation method can be performed alone or in combination. In the case of performing the methods in combination, the avidity is actually calculated for the compounds that has been expected to be more desirable in visual investigation, and the validity thereof is evaluated. By repeatedly performing the calculation and evaluation, more excellent compounds may be designed, identified, evaluated or searched.

Next, the designed, identified, evaluated or searched compound is optimized to be a more excellent compound, such as a compound having more excellent characteristics as a medicament, such as being excellent *in vivo* kinetics, having low toxicity and low side-effect; a compound having a still higher biological activity as an effector; a compound having an advantageous structure as a medicament in view of its oral administration; and the like.

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The resulting candidate compound can be obtained using generally used techniques for chemical synthesis depending on the kind of the compound.

The present invention also encompasses an effector of the dipeptidyl peptidase IV, which is obtained by the method of the present invention for designing, identifying, evaluating or searching an effector. When the effector is a compound capable of inhibiting or enhancing the activity of the dipeptidyl peptidase IV, the effector (inhibitor or activator) is expected to be an agent for, for example, a modulatory agent of immune response, a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like.

The three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention can be provided as a computer program, a medium or the like, which displays the three-dimensional structure of the molecule based on the three-dimensional structural coordinate and can be provided via a telecommunication line or the like. Therefore, using a computer or the like, the three-dimensional coordinate of the dipeptidyl peptidase IV can be displayed in detail, allowing to perform the method of the present invention for designing, identifying, evaluating or searching an effector more rapidly, conveniently and logically.

The present invention also encompasses a program or a medium therefor for use of the three-dimensional structural coordinate, in which all and/or a part of the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention is recorded.

The medium may be any of those in which the three-dimensional structural coordinate of the present invention can be derived on a program that

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runs on a computer, and includes, for instance, electric memory media referred to as memory; semi-permanent memory media such as a FD, a hard disk, an optical disk, an opto-magnetic disk and a magnetic tape, and the like. In addition, the program and the medium therefor for use of the three-dimensional structural coordinate of the present invention also encompass those having a form which can be communicated via a telecommunication line such as internet.

Also, the program and the medium therefor for use of the three-dimensional structural coordinate of the present invention may further comprise a means for displaying the three-dimensional graphic display of the molecule. The program or the medium therefor which comprises the means for displaying the three-dimensional graphic display has advantages that visual studies and/or calculation of avidity can be made more conveniently, so that there is more facilitated a logical design on the three-dimensional structural level for obtaining a compound having excellent characteristics such as higher avidity, higher biological activity, higher biological stability, higher thermomechanical stability, higher absorbency to a living body, and lower toxicity than those for known effectors of the dipeptidyl peptidase IV.

As the means capable of displaying the three-dimensional graphic display, there may be generally used a program that is made so that a means for inputting the three-dimensional structural coordinate of the molecule, a means for measuring visual representation of the coordinate on a computer screen, the distance between the represented atoms in the molecule, bond angles or the like, a means for addition or modification of the coordinate, and the like can be provided. Furthermore, there may be used a program that has been made so that a means for calculating the structure energy of the molecule based on the

coordinate of the molecule, a means for calculating the free energy of bonding, and the ratio of bonding state number to non-bonding state number in consideration of solvent molecules such as water molecule can be provided. Examples of the program suitable for such purposes include Insight II, QUANTA and the like, which are computer programs commercially available from Accelrys Inc., and the present invention is not limited to these programs. Also, the above-mentioned programs can be introduced into a computer referred to as a work station supplied from Silicone Graphics Inc., SunMicro-Systems Ltd., or the like, and used.

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According to the crystal of dipeptidyl peptidase IV of the present invention, there can be exhibited excellent effects that the three-dimensional structural coordinate can be obtained as an information for designing, identifying, evaluating or searching an effector of the dipeptidyl peptidase IV useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like, and that the crystal of a complex of the dipeptidyl peptidase IV and a known effector can be readily prepared. Also, according to the three-dimensional structural coordinate of the present invention, there is exhibited an excellent effect that the effector can be designed, identified, evaluated or searched. In addition, according to the method for obtaining a three-dimensional structural coordinate of the homolog protein of the dipeptidyl peptidase IV of the present invention, there is exhibited an excellent effect that the three-dimensional structural coordinate of the homolog protein of the dipeptidyl peptidase IV of which three-dimensional structure is unknown can be conveniently and rapidly provided. Furthermore, according to the method for

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obtaining a three-dimensional structure of a crystal of a complex of the dipeptidyl peptidase IV of the present invention and an effector of the dipeptidyl peptidase IV, there is exhibited an excellent effect that the method can provide a target for designing an effector useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like, and having excellent characteristics such as higher avidity, higher biological activity, higher biological stability, higher thermomechanical stability, and higher absorbency to a living body. Moreover, according to the method of the present invention for identifying a pharmacophore of the dipeptidyl peptidase IV and the effector of the dipeptidyl peptidase IV, there is exhibited an excellent effect that the method can provide a target for designing the effector useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like, and having excellent characteristics such as higher avidity, higher biological activity, higher biological stability, higher thermomechanical stability, and higher absorbency to a living body. According to the method of the present invention for designing, identifying, evaluating or searching an effector of the dipeptidyl peptidase IV, there is exhibited an excellent effect that the method can logically and conveniently provide an effector useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like, and having excellent characteristics such as higher avidity, higher biological activity, higher biological stability, higher thermomechanical stability,

and higher absorbency to a living body. According to the effector of the dipeptidyl peptidase IV of the present invention, there are exhibited excellent effects that the effector is capable of modifying immune response and capable of treating or preventing diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like. Furthermore, according to the program and medium therefor of the present invention, there is exhibited an excellent effect that the method for designing, identifying, evaluating or searching an effector of the dipeptidyl peptidase IV can be performed more rapidly and conveniently.

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The present invention will be hereinafter more specifically explained by the following Examples, but the present invention is not intended to be limited by the Examples in any way. Unless otherwise indicated, the reaction conditions, procedures and the like can be referred to the instruction manual attached to the reagents used, *Molecular Cloning A Laboratory Manual*, third edition, Sambrook et al. [issued by Cold Spring Harbor Laboratory Press (2001)], and the like.

Example 1 Construction of Recombinant Baculovirus for Expression of Soluble Human Dipeptidyl Peptidase IV

20 (1) Cloning of Soluble Human Dipeptidyl Peptidase IV (shDPPIV) cDNA

Caco-2 cells [provided by American Type Culture Collection (ATCC)]

were cultured at 37°C using Dulbecco's Modified Eagle Medium (manufactured by Invitrogen) containing 20% by volume of inactivated fetal bovine serum (manufactured by Invitrogen; inactivated by incubation at 56°C for 30 minutes)

and 1% by volume of nonessential amino acid (manufactured by Invitrogen), in

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the presence of 5% by volume of CO₂.

Next, total RNA was extracted from the Caco-2 cells obtained.

Extraction of the total RNA was carried out using a product manufactured by

Nippon Gene Co. Ltd. under the trade name of ISOGEN in accordance with the

attached instruction manual. The obtained total RNA was used as a template for

RT-nested PCR method described below.

In order to obtain a nucleic acid corresponding to a soluble human DPPIV from which the signal peptide sequence was removed (amino acid nos: 33-766 of SWISS-PROT Accession No: P27487), first, a cDNA fragment sequence of human DPPIV gene was amplified by RT-nested PCR method with total RNA of the Caco-2 as a template.

The thermal profile in the PCR is 30 cycles of reaction, in which one cycle comprises denaturation at 94°C for 30 seconds, annealing at 55°C for 30 seconds and polymerase extension reaction at 72°C for 1 minute.

The amplified DNA fragment was separated by agarose gel electrophoresis method, and a small fragment of the gel of the corresponding band portions was cut out. Thereafter, the DNA fragment was extracted from the obtained small fragments of the gel using a product manufactured by Bio 101 under the trade name of GENE CLEAN SPIN Kit, and purified. The obtained fragment was inserted into vector pCR2.1-TOPO contained in TOPO TA Cloning (registered trade mark) Kit manufactured by Invitrogen to construct pCR-shDPPIV.

In order to confirm whether or not the obtained cDNA fragment encodes the desired polypeptide, deletion mutants regarding the DNA fragment having various lengths were prepared, and a nucleotide sequence for the DNA fragment

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was determined as follows.

First, a DNA fragment having a size of 2.2 kbp obtained by double digestion of the pCR-shDPPIV with BamHI and EcoRI was inserted into a corresponding restriction site in pUC19 (manufactured by Takara Bio Inc.), to construct a plasmid pUshDPPIV. Various deletion plasmids were prepared using the plasmid pUshDPPIV by a conventional method.

The nucleotide sequence for the DNA fragment was determined using the obtained deletion plasmid or plasmid pCR-shDPPIV, and a product manufactured by Perkin-Elmer Cetus Inc. under the trade name of Taq DyeDeoxy Terminator Cycle Sequencing Kit and Model 373S sequencer manufactured by Applied Biosystems.

Also, the amino acid sequence of the polypeptide encoded by the abovementioned DNA fragment was determined on the basis of the nucleotide sequence.

The determined amino acid sequence was compared with the sequence for a full length DPPIV of human colon shown in SEQ ID NO: 2. As a result, it was confirmed that the corresponding regions (regions excluding the transmembrane region) were identical.

Thus, it was confirmed that the DNA fragment encodes the desired polypeptide shDPPIV, namely a polypeptide in which the transmembrane region (amino acid nos: 1-32 at N-terminal side) in the full-length human DPPIV was deleted and a polyhistidine peptide was added to the C-terminal side.

(2) Preparation of Recombinant Baculovirus

Plasmid pUshDPPIV was digested with a restriction enzyme to give a

DNA fragment encoding shDPPIV gene. The obtained fragment was inserted into pAcGP67B (manufactured by BD PharMingen) to construct a baculovirus transfer vector pAcGP67B-shDPPIV.

Fifteen minutes before the transfection, Sf21 cells were washed twice with a TNM-FH medium comprising 10% by volume of fetal bovine serum. The Sf21 cells were then transferred to a well of a 6-well plate by 2.4×10^6 cells per well.

Furthermore, 2 to 5 µg of the baculovirus transfer vector and a 0.5 µg linear baculovirus DNA (trade name: BaculoGold virus DNA, manufactured by BD PharMingen) were mixed, and the mixture was allowed to stand at room temperature for 5 minutes. Next, 1 ml of Transfection Buffer B (manufactured by BD PharMingen) was added to the obtained mixture, and the mixture was thoroughly mixed to give a Transfection Buffer B/DNA mixture.

The medium in the wells of the 6-well plate and the cells that had not been adhered to the wells were removed, and 1 ml of Transfection Buffer A (manufactured by BD PharMingen) was added to each of the wells. The Transfection Buffer B/DNA mixture was gradually added dropwise to the wells of the 6-well plate, with gently stirring the 6-well plate. The cells were incubated at 28°C for 4 hours in the wells of the 6-well plate. Thereafter, the transfection buffer was removed, and 3 ml of TNM-FH medium containing 10% by volume of fetal bovine serum was added to the wells of the 6-well plate. The cells were cultured at 28°C in each of the wells of the 6-well plate for 5 days, and the culture supernatant was collected. The culture supernatant was used for amplification of virus using Sf21 cells to give a virus stock solution.

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Example 2 Preparation and Crystallization of shDPPIV

(1) Expression of shDPPIV in Insect Cells

Sf21 cells were cultured using a serum free medium EX-CELL 400 (manufactured by JRH Biosciences) and T flask, and Tn5 cells (provided by Invitrogen) were cultured using a serum free medium EX-CELL 401 (manufactured by JRH Biosciences) and a T flask, at 28°C, respectively. At the time when the proliferation of the cells reached 70% confluent, the old medium was removed, and a fresh medium was added at 40 ml per one 225-cm² flask. Then, 1.5 ml of virus stock solution after amplification for three times (having multiplicity of infection (MOI) of about 2) was added to the cells to infect the cells, and the cells were incubated at 28°C for 4 days. The culture supernatant four days after the infection was collected and stored at -20°C. The culture supernatant was used for the purification of shDPPIV protein as described below.

15 (2) Purification of shDPPIV Protein

In each step for the purification of shDPPIV, the activity of DPPIV was measured by incubating a 0.1 ml reaction mixture containing a 1.5 mM substrate [manufactured by Peptide Institute, Gly-Pro-paranitroanilide (pNA)], 71 mM Gly-NaOH (pH 8.7) and the DPPIV, and detecting the liberated pNA.

Meanwhile, the reaction mixture was incubated at 37°C for 10 minutes. During the incubation, the absorbance at 405 nm was monitored.

Also, the protein concentration was quantified by using a product manufactured by Bio-Rad Laboratories, Inc. under the trade name of DC protein Assay Kit II.

The purity of the protein was confirmed by subjecting a protein sample

in each step to SDS-PAGE using 7.5% polyacrylamide gel according to the method by Laemmli et al.

The culture supernatant stored at -20°C in the above-mentioned (1) was melted at 4°C and filtered with a bottle top filter (manufactured by Becton, Dickinson and Company) or with 0.45 µm filter (KURABO INDUSTRIES LTD.) to remove insoluble materials. The supernatant after the filtration was concentrated to an about tenth volume by using a concentrator Vivaflow 50 (manufactured by Sartorius AG) or Amicon stirrer cell model 8400 (manufactured by Millipore Corporation) to give a concentrated solution.

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The obtained concentrated solution was dialyzed against buffer A (20 mM HEPES-NaOH, 0.5 M NaCl, pH 8.0) at 4°C overnight, and applied to a nickel column [one in which nickel was immobilized to HiTrap Chelating column (trade name, manufactured by Amersham-Pharmacia) (5 ml × 2)] equilibrated with buffer A. The column was washed with 10 column volumes of buffer A, and then with buffer A containing 50 mM imidazole. The elution of the fraction containing shDPPIV was carried out by a linear gradient of 50 to 500 mM imidazole. The fraction found to have DPPIV activity was collected, and dialyzed overnight at 4°C against buffer B (20 mM HEPES-NaOH, pH 8.0, 50 mM NaCl). After the dialysis, the sample was purified by using an anion exchange column [manufactured by Amersham-Pharmacia under the trade name: Resource Q (6 ml)] equilibrated with buffer B. The column was washed with buffer B, and thereafter shDPPIV was eluted by a linear gradient of 15 column volumes of 50 to 500 mM NaCl. The fractions found to have DPPIV activity were collected, and used as a purified preparation.

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(3) Preparation of Protein Sample for Crystallization

The shDPPIV purification sample (9 ml) obtained in the above (2) was concentrated using a product manufactured by Millipore Corporation under the trade name of Centricon 10 until the protein concentration reached 10 mg/ml.

The obtained product was used as a protein sample for crystallization. The protein sample for crystallization was stored at 4°C.

A precipitation agent solution containing 0.18 M glycine-NaOH (pH 9.5), 0.18 M sodium sulfate and 18% by weight of PEG4000, and a 10 mg/ml dipeptidyl peptidase IV solution were mixed, and thereafter, a drop of the obtained mixed solution was placed on a product under the trade name of Cryschem Plate (manufactured by Hampton Research). The above-mentioned precipitation solution was allowed to stand at 20°C as a reservoir solution to allow crystallization.

15 (4) Crystallization of shDPPIV

The crystallization of shDPPIV was carried out by a sitting-drop method, which is one of vapor diffusion methods.

The formation of crystal was observed with the passage of time using a stereoscopic microscope. As a result, after about two weeks, a large crystal having a maximum size of 500 μ m \times 300 μ m \times 100 μ m was obtained. The crystal is also referred to as a native crystal. The microphotograph of the obtained crystal is shown in Figure 1. In Figure 1, the visual field is 4000 μ m \times 3000 μ m.

25 Example 3 Three-Dimensional Structural Analysis of Crystals

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(1) X-ray Diffraction

The crystal obtained in Example 2 mentioned above was soaked in a cryoprotecting buffer [composition: 0.18 M glycine-NaOH (pH 9.5), 19% by weight of PEG4000, 0.18 M sodium acetate, 15% glycerol], and immediately thereafter the mixture was placed under nitrogen gas stream (100 K) to rapidly freeze the mixture.

The X-ray diffraction intensity data of the above crystal were collected up to the resolution of 3.0Å using a product manufactured by Rigaku International Corporation under the trade name of R-AXIS IV in nitrogen gas stream (100 K), and converted to the structure factor using a program MOSFLM (Version 6.11). A photograph of the diffraction pattern is shown in Figure 2.

From the obtained diffraction intensity data, it was determined that the crystal form to which the crystal belongs was orthorhombic, that the space group was $P2_12_12_1$, and the lattice constants were $a = 118.0 \pm 5.0$ Å, $|b| = 125.9 \pm 5.0$ Å and $|c| = 136.8 \pm 5.0$ Å.

(2) Multiple Isomorphous Replacement Method

In order to derive an electron density map, multiple isomorphous replacement method was carried out. The crystal obtained in Example 2 was soaked for 3 days and 4 days in a crystallization solution prepared by dissolving mercury chloride until being saturated, to give two different kinds of isomorphous replacement crystals containing mercury atoms in the crystals. The X-ray diffraction intensity data were collected in the same manner as those for the native crystals.

In the determination of the phase in the structural analysis, CCP4

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(Collaborative Computational Project, Number 4, 1994. "The CCP4 Suite: Programs for Protein Crystallography," *Acta Cryst.* D50, 760-763) program was used.

First, Fourier transform calculation utilizing the difference between the diffraction intensity obtained from the two kinds of isomorphous replacement crystals of mercury and the diffraction intensity obtained from the native crystal was performed using MLPHERE contained in the CCP program package. The position of each mercury atom in the unit cell of the real space was determined by investigating large peaks provided by heavy atoms (mercury) in the obtained Patterson's diagram. The phase of the crystal structure factor of the native crystals was determined by using the obtained position coordinate of mercury atoms. Furthermore, in order to determine the coordinate of each mercury atom more accurately using DM and SOLOMON contained in the CCP program package, refinement was carried out using three crystal structure factors of the native crystals and of the two kinds of mercury isomorphous replacement crystals.

An electron density map of the crystals of the dipeptidyl peptidase IV in real space was obtained using the phase of the crystal structure factor of the native crystals calculated from the refined coordinates of the mercury atoms. Furthermore, the electron density map was improved by carrying out smoothening and histogram matching of the electron density map in a solvent region, to obtain an electron density map critical for molecular modeling.

(3) Molecular Modeling

The sites corresponding to the amino acid residues of the dipeptidyl

peptidase IV were identified on the electron density map by using QUANTA (manufactured by Accelrys, Inc.), to build molecular models.

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As expected from the lattice constants, there were two molecules of the dipeptidyl peptidase IV in an asymmetry unit, and a model was built for each of the molecules. The refinement of the obtained molecular model was carried out using CNX (manufactured by Accelrys, Inc.), and the molecular model was adjusted again using the QUANTA for the obtained improved electron density map. The procedures were repeated to build a more accurate molecular model. In the refinement of the final coordinate, diffraction intensity data measured again were used after OSMIC confocal mirror (manufactured by Rigaku International Corporation) had been introduced into R-AXIS IV (trade name, manufactured by Rigaku International Corporation).

As a result, the resolution was improved from the previous 3.0Å to 2.6Å. Furthermore, 273 molecules of bound water and 5 molecules of N-acetyl glucosamine residues per molecule of the dipeptidyl peptidase IV were identified in an asymmetric unit. R factor, which is an index for accuracy of the obtained molecular model, was 24.89%, and a free R factor, which independently was not taken into account of the calculation of refinement at the step of refinement, was 30.15%. During the procedure, the deviation of the interatomic bond distance (rms-deviation) and the bond angle from the ideal state of the three-dimensional structure were 0.006Å and 1.305°, respectively. The stereogram of the three-dimensional structure model of the crystals is shown in Figure 3, and the coordinate is shown in Figure 4. The present coordinate data were registered in PDB (Brookhaven Protein Data Bank) [PDB Code No: 1J2E, RSCB code No: 005544].

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Here, as to those regions which did not take a regular structure in the crystals (in the disordered state), namely, the region from Asp 38 to that closer to the N-terminal side thereof, and the region for the tagged peptide (polyhistidine peptide) of the C-terminal side, the molecular model could not be built.

Furthermore, a part of the side chains projected to the surface of the molecules did not take a regular structure. However, these residues were not portions that play an important role for the function of enzymes.

In the three-dimensional structure of the dipeptidyl peptidase IV, which has been clarified by the Examples, it has been revealed that the amino acid residue involved in the activity deduced by various experiments for the dipeptidyl peptidase IV, namely, Ser 630, Asp 708 and His 740, form hydrogen bonds between the $O_{\delta 2}$ atom of Asp 708 and $N_{\delta 1}$ atom of His 740, and with the $N_{\epsilon 2}$ atom of His 740 and O_{γ} atom of Ser 630, even the residues locate in distant locations on the primary sequence. Therefore, for the structural coordinate of Figure 4 and the three-dimensional structure model defined by the structural coordinate, it is suggested that the regions characterized by Ser 630, Asp 708 and His 740, and the whole or a part of amino acid residues that are located in the vicinity of Ser 630, Asp 708 and His 740 play an important role on the exhibition of the activity for the dipeptidyl peptidase IV and binding or interaction of the dipeptidyl peptidase IV with the effector, and that the compound matching the three-dimensional structure of the regions affect the activity for the dipeptidyl peptidase IV.

The present invention may be embodied in other various forms without departing from the spirit or essential characteristics thereof. The present

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embodiment is therefore to be considered in all respects as illustrative and not restrictive, the scope of the invention being indicated by the appended claims rather than by the foregoing description and all changes which come within the meaning and range of equivalency of the claims are therefore intended to be embraced therein.

INDUSTRIAL APPLICABILITY

According to the crystal of the dipeptidyl peptidase IV of the present invention, the information of a three-dimensional structure coordinate suitable for designing, identifying, evaluating or searching an effector of the dipeptidyl peptidase IV, useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like can be obtained. Also, according to the three-dimensional structure coordinate, the information of a three-dimensional structure coordinate suitable for designing, identifying, evaluating or searching an effector of the dipeptidyl peptidase IV, useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like can be obtained. Further, according to the method of the present invention for obtaining a threedimensional structure coordinate of a homolog protein of a dipeptidyl peptidase IV, the refinement of the three-dimensional structure coordinate of the homolog protein of the dipeptidyl peptidase IV can be more conveniently carried out. Moreover, according to the method of the present invention for obtaining a threedimensional structure coordinate of a crystal of a complex of a dipeptidyl

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peptidase IV with an effector of the dipeptidyl peptidase IV, the information of a three-dimensional structure coordinate suitable for designing, identifying, evaluating or searching an effector of the dipeptidyl peptidase IV, which is useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like, and is excellent in avidity, biological activity, biological stability, absorbency to a living body, and which can favorably act on the dipeptidyl peptidase IV can be obtained. Also, according to the method for identifying a pharmacophore of a dipeptidyl peptidase IV and an effector of the dipeptidyl peptidase, the information of a three-dimensional structure coordinate suitable for designing, identifying, evaluating or searching an effector of the dipeptidyl peptidase IV, which is useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like, and is excellent in avidity, biological activity, biological stability, absorbency to a living body, and which can favorably act on the dipeptidyl peptidase IV can be obtained. Further, according to the method of the present invention for designing, identifying, evaluating or searching an effector of the dipeptidyl peptidase IV, the information of a three-dimensional structure coordinate suitable for designing, identifying, evaluating or searching an effector of the dipeptidyl peptidase IV, which is useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like, and is excellent in avidity, biological activity, biological stability, absorbency to a living body,

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and which can favorably act on the dipeptidyl peptidase IV can be logically and conveniently obtained. In addition, the effector of the dipeptidyl peptidase IV of the present invention is useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like. Further, according to the program or the medium therefor of the present invention, the design, identification, evaluation and search for an effector of a dipeptidyl peptidase IV can be carried out rapidly and conveniently. Therefore, the present invention can be utilized in modulation of immune response and the treatment or prevention for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like.

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CLAIMS

- 1. A crystal of a dipeptidyl peptidase IV, having characteristics sufficient to ensure a resolution capable of analyzing its three-dimensional structure up to the side chain level by X-ray crystallographic structural analysis.
- 2. The crystal according to claim 1, wherein the dipeptidyl peptidase IV is a soluble polypeptide comprising a region located at extramembrane in a full-length human dipeptidyl peptidase IV.

3. The crystal according to claim 1 or 2, wherein the dipeptidyl peptidase IV is a polypeptide having an amino acid sequence in which a transmembrane region is deleted from the amino acid sequence of SEQ ID NO: 2, and a tag peptide is optionally added to a C-terminal side or N-terminal side thereof.

4. The crystal according to any one of claims 1 to 3, wherein the crystal has a space group of $P2_12_12_1$, and a lattice constant of the unit cell of $|a| = 118.0 \pm 5.0$ Å, $|b| = 125.9 \pm 5.0$ Å, $|c| = 136.8 \pm 5.0$ Å, and $\alpha = \beta = \gamma = 90^{\circ}$, and is orthorhombic.

- 5. The crystal according to any one of claims 1 to 4, wherein the crystal has the structural coordinate shown in Figure 4.
- 6. The crystal according to any one of claims 1 to 4, wherein the crystal has a structural coordinate different from the structural coordinate as shown in

Figure 4 via fluctuation of a protein.

7. A three-dimensional structural coordinate of a dipeptidyl peptidase IV, comprising the structural coordinate shown in Figure 4.

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8. A three-dimensional structural coordinate of a dipeptidyl peptidase IV, comprising a structural coordinate different from the structural coordinate as shown in Figure 4 via fluctuation of a protein.

9. The three-dimensional structural coordinate according to claim 8, wherein the fluctuation of a protein is a state that is caused by molecular oscillation or temperature, and exhibits an activity for the dipeptidyl peptidase IV in a living

body.

15 10. The three-dimensional structural coordinate according to any one of claims 7 to 9, wherein the dipeptidyl peptidase IV is a soluble polypeptide comprising a region located at extramembrane in a full-length human dipeptidyl peptidase IV.

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11. The three-dimensional structural coordinate according to any one of claims 7 to 10, wherein the dipeptidyl peptidase IV is a polypeptide having an amino acid sequence in which a transmembrane region is deleted from the amino acid sequence of SEQ ID NO: 2, and a tag peptide is optionally added of to a C-terminal side or N-terminal side thereof.

- 12. A three-dimensional structural coordinate of a region in a dipeptidyl peptidase IV, comprising the three-dimensional structural coordinate of the region selected from the group consisting of the following (a) to (d):
- (a) a region characterized by Ser 630, Asp 708 and His 740 in the amino acid sequence of SEQ ID NO: 2, and all or a part of a group of the amino acid residues located in the adjacent area of each of the Ser 630, Asp 708 and His 740 in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural coordinate;
- 10 (b) a region characterized by Ser 630, Asp 708 and His 740 in the amino acid sequence of SEQ ID NO: 2, and all or a part of a group of the amino acid residues comprising amino acids capable of maintaining physicochemical characteristics physiologically equivalent to each of amino acids in the group of the amino acid residues located in the adjacent area of each of Ser 630, Asp 708 and His 740, in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural coordinate,
- (c) a region characterized by a group of amino acid residues comprising amino acids capable of maintaining physicochemical characteristics

 20 physiologically equivalent to each of Ser 630, Asp 708 and His 740 in the amino acid sequence of SEQ ID NO: 2, and all or a part of a group of the amino acid residues located adjacent area of said group of the amino acid residues in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural coordinate; and

(d) a region characterized by a group of amino acid residues comprising amino acids capable of maintaining physicochemical characteristics physiologically equivalent to each of Ser 630, Asp 708 and His 740 in the amino acid sequence of SEQ ID NO: 2, and

5 all or a part of a group of amino acid residu

all or a part of a group of amino acid residues comprising amino acids capable of maintaining physicochemical characteristics physiologically equivalent to each of the amino acids in the group of the amino acid residues located in the adjacent area of said group of the amino acids, in the structural coordinate shown in Figure 4 or the three-dimensional

structure model defined by the structural coordinate,

wherein the region in the dipeptidyl peptidase IV is a region involved in binding or interaction between the dipeptidyl peptidase IV and an effector of the dipeptidyl peptidase IV.

- 13. The three-dimensional coordinate according to claim 12, wherein the physicochemical characteristic is selected from the group consisting of features in shape of a three-dimensional structure, hydrophobicity, electric charge and pK.
- 14. A method for obtaining a three-dimensional coordinate of a homolog
 20 protein of a dipeptidyl peptidase IV, characterized in refining an electron density map of the homolog protein of the dipeptidyl peptidase IV comprising the amino acid sequence of SEQ ID NO: 2, based on all and/or a part of the three-dimensional coordinate of any one of claims 7 to 13, to give a three-dimensional structural coordinate.

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- 15. A method for obtaining a three-dimensional structural coordinate of a crystal of a complex of a dipeptidyl peptidase IV and an effector of the dipeptidyl peptidase IV characterized in using all and/or a part of the three-dimensional structural coordinate of any one of claims 7 to 13, to give a three-dimensional structural coordinate.
- 16. A method for identifying pharmacophore of an effector of the dipeptidyl peptidase IV, characterized in identifying the pharmacophore based on all and/or a part of the three-dimensional structural coordinate of any one of claims 7 to 13, and the steric conformation of the effector of the dipeptidyl peptidase IV.
- 17. A method for designing, identifying, evaluating or searching an effector of a dipeptidyl peptidase IV, characterized in designing, identifying, evaluating or searching a compound capable of acting on the dipeptidyl peptidase IV, based on all and/or a part of the three-dimensional structural coordinate of any one of claims 7 to 13.
- 18. The method according to claim 17, wherein the method for designing, identifying, evaluating or searching an effector comprises the steps of:
- 20 (i) identifying a region to be targeted for binding or interaction with the effector in a dipeptidyl peptidase IV, based on all and/or a part of the three-dimensional structural coordinate according to any one of claims 7 to 13 and the steric conformation of the effector of the dipeptidyl peptidase IV;
- 25 (ii) identifying atoms or atomic groups capable of generating in the above

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region at least one intermolecular interaction selected from the group consisting of covalent bond, ionic interaction, ion-dipole interaction, dipole-dipole interaction, hydrogen bonding, van der Waals force, electrostatic interaction and hydrophobic interaction, with the atoms or atomic groups existing in a candidate compound; and

- (iii) designing a compound based on the information of the above step (i) and/or (ii).
- 19. The method according to claim 18, wherein the method further comprisesthe steps of:

detecting an interaction between the dipeptidyl peptidase IV and the designed, identified, evaluated or searched candidate compound, wherein when an interaction is detected, the candidate compound is identified as a compound capable of binding to the dipeptidyl peptidase IV, based on a degree of the interaction as an index.

20. The method according to claim 18 or 19, wherein the method further comprises the steps of:

contacting the dipeptidyl peptidase IV with the designed, identified,

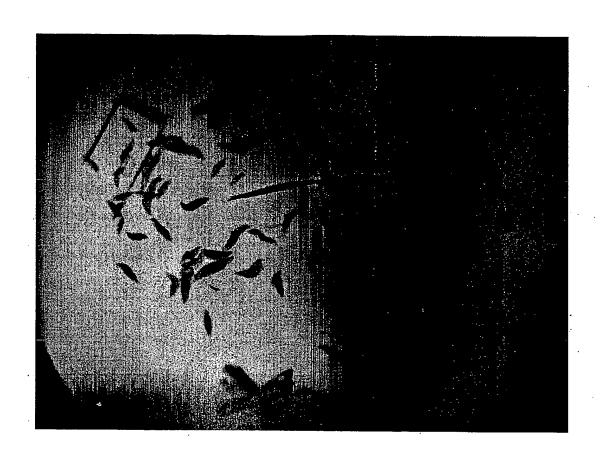
evaluated or searched candidate compound and measuring an activity of the
dipeptidyl peptidase IV,
wherein when an activity increases or decreases, the designed, identified,
evaluated or searched candidate compound is identified as a compound having
enhancing action or inhibitory action on the activity of the dipeptidyl peptidase

IV, based on a degree of the increase or decrease as an index.

- 21. An effector of the dipeptidyl peptidase IV obtainable by the method of any one of claims 17 to 20.
- 5 22. A program and a medium therefor for use of the three-dimensional structural coordinate of any one of claims 7 to 13, wherein all and/or a part of the three-dimensional structural coordinate of any one of claims 7 to 13 is recorded.
- 23. The program and the medium according to claim 22, comprising a means for identifying, searching, evaluating or designing a compound capable of binding to the dipeptidyl peptidase IV or a compound having an enhancing action or inhibitory action on the activity for the dipeptidyl peptidase IV.
- The program and the medium according to claim 23, further comprising a
 means for displaying a three-dimensional graphic display of a molecule.

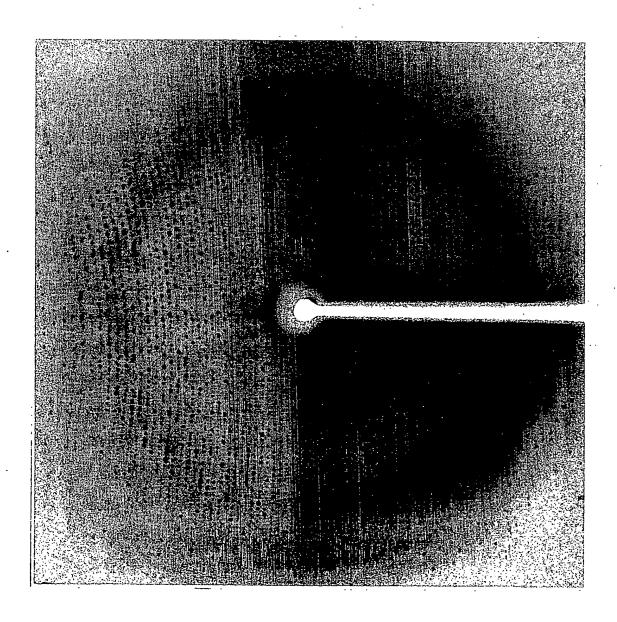
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FIG. 1



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FIG. 2



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FIG. 3

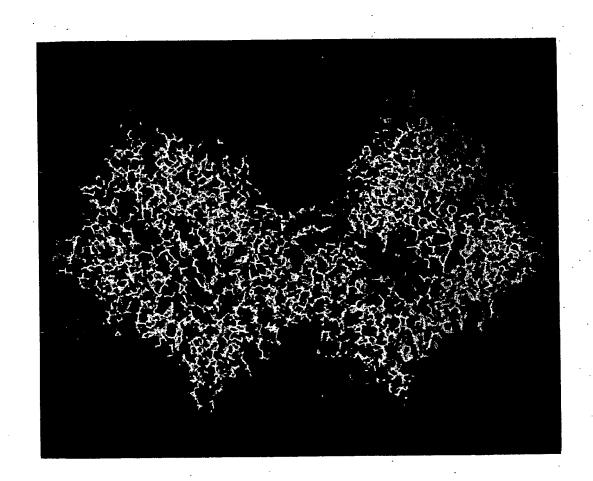


FIG. 4-1

	Th	ree-	-dime	nsional	structural	coordin	nate of	dipeptidyl p	eptidase	IV
ATOM	1	СВ	ASP	38	44. 493	31.885	58. 927	1.00 42.46	S A	С
ATOM	2	CG	ASP	38	44. 146	32.095	57. 467			č
ATOM	3	0D1	ASP	38	43.664	33. 198	57. 133			ő
ATOM	4	0D2		38	44.360	31.171	56. 655			ŏ
ATOM	5	C	ASP	38	45. 876	29. 805	58. 634			č
ATOM	6	0	ASP	38	46.980	30. 327	58. 778			ŏ
ATOM	7	N	ASP	38	44. 758	30. 264	60. 778			N
ATOM	8	CA	ASP	38	44.639	30. 404	59. 296			Ċ
ATOM	9	N	SER	39	45.679	28.711	57.905			Ň
ATOM	10	CA	SER	39	46.775	28.013	57. 241			Ĉ
ATOM	11	CB	SER	39	46.584	26.501	57. 380			Č
ATOM	12	0G	SER	39	45.410	26.079	56. 703			0
ATOM	13	C	SER	39	46.960	28.343	55.763			C
ATOM	14	0	SER	39	47.870	27.813	55. 123			0
ATOM	15	N	ARG	40	46.093	29.190	55. 217	1.00 38.12		N
ATOM	16	CA	ARG	40	46. 194	29.575	53.810	1.00 37.02		C
ATOM	17	CB	ARG	40	45.082	30.558	53.439	1.00 36.96		C
ATOM	18	CG	ARG	40	43.683	29.984	53.404		A	C
ATOM	19	CD	ARG	40	42.688	31.098	53. 137	1.00 34.97	Α	C
ATOM	20	NE	ARG	40	42.774	32.134	54. 161	1.00 35.27		N
ATOM	21	CZ	ARG	40	42.097	33. 276	54. 125			C
ATOM	22		ARG	40	41. 280	33. 528	53. 111	1.00 35.54		N
ATOM		NH2		40	42. 239	34. 167	55.097		Α	N
ATOM	24		ARG	40	47. 530	30. 251	53. 531	1.00 35.91	A	C
ATOM			ARG	40	48. 100	30.901	54. 407	1.00 34.18	A	0
ATOM ATOM			LYS	41	48. 031	30.100	52. 310	1.00 35.43	A	N
ATOM			LYS	41	49. 286	30.749	51.937	1.00 34.97	A	C
ATOM			LYS LYS	41	49. 705	30. 338	50. 525	1.00 35.73	A	C
ATOM			LYS	41 41	48. 684	30.719	49.467	1.00 38.56	A	C
ATOM			LYS	41	49. 026 47. 805	30. 151	48.096	1.00 42.36	A	C
ATOM			LYS	41	48. 070	30. 201 29. 686	47. 173 45. 791	1.00 45.55	A	C
ATOM			LYS	41	49.038	32. 257		1.00 47.41	A	N
ATOM			LYS	41	47. 891	32. 715	51.957 51.981	1.00 33.41 1.00 33.24	A	C
ATOM			THR	42	50.110	33. 032	51. 954	1.00 33.24 1.00 31.47	A	0
ATOM			THR	42	49. 967	34. 479	51. 937	1.00 31.47	A	N
ATOM			THR	42	50. 860	35. 139	53.000	1.00 30.04	A	C
ATOM			THR	42	52. 234	34. 843	52. 725	1.00 31.23	A A	C
ATOM			THR	$\frac{\tilde{42}}{42}$	50. 501	34. 622	54. 386	1.00 30.13	A	C 0
ATOM			THR	42	50. 389	34. 971	50. 558	1.00 28.34	A	Č
ATOM			THR	42	50. 977	34. 220	49. 782	1.00 27.76	A	Õ
ATOM	42		TYR	43	50.058	36. 217	50. 234	1.00 27.55	A	N .
ATOM	43		TYR	43	50.465	36. 782	48. 954	1.00 25.72	A	Č
ATOM			TYR	43	49. 615	38. 006	48. 623	1.00 26.01	A	Č
ATOM	45		TYR	43	49. 922	38. 625	47. 280	1.00 26.92	A	Č
ATOM	46		TYR	43	50.977	39.527	47. 130	1.00 26.68	A	č
ATOM			TYR	43	51.253	40.113	45.895	1.00 27.02	A	č
ATOM	48	CD2	TYR	43	49. 152	38. 315	46.158	1.00 26.40	A	č
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(Continued)

F	Т	\boldsymbol{C}	1	_	9
г	1	U.	4		4

	40	ODO	TV.	40	40 404	20 001	44.919	1.00 25.89	Α	C
ATOM	49		TYR	43	49. 424	38. 891				Č
ATOM	50	CZ	TYR	43	50. 473	39. 790	44. 796	1.00 25.91	A	
ATOM	51	OH	TYR	43	50. 741	40.370	43.579	1.00 25.09	A	0
ATOM	52	C	TYR	43	51.933	37. 165	49.160	1.00 24.97	A	C
ATOM	53	0	TYR	43	52. 251	38.049	49.955	1.00 23.33	· A	0
ATOM	54	N	THR	44	52.818	36.482	48.444	1.0024.06	Α	N
ATOM	55	CA	THR	44	54. 255	36.685	48.580	1.00 25.90	Α	С
ATOM	56	CB	THR	44	54.960	35. 336	48. 547	1.00 25.86	A	С
	57	0G1	THR	44	54.696	34. 709	47. 285	1.00 28.12	Ā	Õ
ATOM			THR	44	54. 439	34. 436	49.655	1.00 22.61	Ä	Č
ATOM	58					37.576	47. 530	1.00 27.35	Ä	Č
ATOM	59	C	THR	44	54.917					Õ
ATOM	60	0	THR	44	54. 296	37. 956	46. 535	1.00 29.11	A	
ATOM	61	N	LEU	45	56. 191	37.894	47. 765	1.00 27.39	A	N
ATOM	62	CA	LEU	45	56. 978	38.722	46.853	1.00 26.43	A	C
ATOM	63	CB	LEU	45	58. 377	38.954	47.425	1.00 26.07	A	C
ATOM	64	CG	LEU	45	59. 310	39.860	46.612	1.00 26.21	A	C
ATOM	65	CD1		45	58.734	41.263	46.517	1.00 25.53	· A	C
ATOM	66	CD2		45	60.672	39.896	47. 266	1.00 24.37	Α	C
ATOM	67	C	LEU	45	57. 088	38.069	45.473	1.00 27.00	· A	C
ATOM	68	ŏ	LEU	45	56. 939	38. 740	44. 449	1.00 27.84	A	0
ATOM	69	N	THR	46	57. 354	36.766	45. 445	1.00 26.70	Ä	N.
		CA	THR	46	57.448	36.038	44. 182	1.00 26.95	A	Ċ
ATOM	70					34. 559	44. 407	1.00 26.87	A	Č
ATOM	71	CB	THR	46	57. 838			1.00 20.87		0
ATOM	72	0G1	THR	46	59. 150	34. 495	44.966		A	C
ATOM	73	CG2	THR	46	57.833	33. 793	43.110	1.00 28.08	A	
ATOM	74	C	THR	46	56.076	36.091	43.517	1.00 26.96	A	C
ATOM	75	0	THR	46	55.965	36.094	42. 289	1.00 25.36	A	0
ATOM	76	N	ASP	47	55.035	36. 126	44. 346	1.00 27.72	A	N
ATOM	77	CA	ASP	47	53.659	36. 199	43.858	1.00 29.74	A	C
ATOM	78	CB	ASP	47	52.670	36. 173	45.026	1.00 30.90	A	C
ATOM	79	CG	ASP	47	52.289	34. 769	45. 430	1.00 30.62	A	C
ATOM	80	0D1	ASP	47	51.778	34. 595	46.553	1.00 32.28	A	0
ATOM	81	0D2	ASP	47	52. 490	33. 845	44.617	1.00 30.71	A	0
ATOM	82	C	ASP	47	53.477	37.482	43.073	1.00 28.87	, A	C
ATOM	83	0	ASP	47	52.918	37.478	41.979	1.00 29.50	A	0
ATOM	84	N	TYR	48	53.945	38. 581	43.648	1.00 28.54	Α	N
ATOM	85	CA	TYR	48	53.859	39.878	42.994	1.00 29.04	A	C
ATOM	86	CB	TYR	48	54. 191	40.991	43.996	1.00 27.50	\mathbf{A}_{\cdot}	C
ATOM	87	CG	TYR	48	54. 448	42. 333	43.354	1.00 25.16	A [*]	C
ATOM	88	CD1		48	53. 460	42.971	42.609	1.00 23.19	Α	C
ATOM	89		TYR	48	53. 703	44. 184	41.982	1.00 24.84	A	Č
ATOM	90		TYR	48	55. 694	42. 946	43. 461	1.00 25.89	Ä	Č
ATOM	91		TYR	48	55. 956	44. 165	42. 838	1.00 26.76	Ä	Č
					54. 955	44. 779	42. 096	1.00 27.28	Ä	Č
ATOM	92	. CZ	TYR	48				1.00 27.28	A	Õ
ATOM	93	· OH	TYR	48	55. 208	45.977	41.463		A	C
ATOM	94	C	TYR	48	54. 820	39. 953	41. 796	1.00 28.80		
ATOM	95	0	TYR	48	54. 445	40.401	40.714	1.00 28.24	A	0
ATOM	96	N	LEU	49	56.054	39. 499	41.988	1.00 29.41	A	N
ATOM	97	CA	LEU	49	57.046	39. 552	40.918	1.00 30.39	Α	С

					FΙ	G. 4	- 3			(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	98 99 100 101 102 103 104		LEU LEU LEU LEU LEU LEU LEU	49 49 49 49 49 49	58. 455 58. 988 60. 438 58. 860 56. 804 57. 147 56. 198	39. 318 40. 473 40. 223 41. 773 38. 606 38. 919 37. 459	41. 481 42. 336 42. 711 41. 555 39. 752 38. 614 40. 024	1.00 27.73 1.00 28.28 1.00 26.99 1.00 26.02 1.00 30.71 1.00 30.14 1.00 32.51	A A A A A	C C C C C O N
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	105 106 107 108 109 110 111	CA CB CG CD CE NZ C	LYS LYS LYS LYS LYS LYS LYS	50 50 50 50 50 50 50	55. 959 56. 289 57. 763 58. 591 60. 071 60. 859 54. 572	36. 491 35. 098 34. 940 35. 213 34. 945 35. 028 36. 517	38. 971 39. 485 39. 790 38. 545 38. 778 37. 515 38. 361	1. 00 33. 54 1. 00 33. 30 1. 00 33. 89 1. 00 35. 19 1. 00 38. 12 1. 00 39. 27 1. 00 34. 93 1. 00 35. 13	A A A A A	C C C C C N C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	112 113 114 115 116 117 118 119	ND2 C	LYS ASN ASN ASN ASN ASN ASN	50 51 51 51 51 51 51	54. 272 53. 731 52. 379 52. 428 53. 407 53. 212 54. 470 51. 529	35. 719 37. 436 37. 569 37. 859 38. 968 40. 131 38. 609 36. 324	37. 478 38. 822 38. 294 36. 791 36. 436 36. 801 35. 717 38. 517	1. 00 36. 66 1. 00 38. 39 1. 00 41. 61 1. 00 44. 75 1. 00 46. 38 1. 00 45. 80 1. 00 38. 21	A A A A A A	N C C C O N C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	120 121 122 123 124 125 126 127	O N CA CB OG1 CG2 C	ASN THR THR THR THR THR THR	51 52 52 52 52 52 52 52	50. 708 51. 720 50. 942 51. 297 52. 646 50. 367 49. 431 48. 699	35. 976 35. 647 34. 451 33. 888 33. 415 32. 750 34. 686 33. 889	37. 674 39. 641 39. 926 41. 298 41. 272 41. 666 39. 869 39. 276	1.00 40.60 1.00 36.74 1.00 35.44 1.00 35.57 1.00 38.62 1.00 35.25 1.00 35.17 1.00 36.44	A A A A A A	0 N C C O C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	128 129 130 131 132 133 134 135	N CA CB CG CD1 CE1 CD2	TYR TYR TYR TYR TYR TYR TYR	53 53 53 53 53 53 53	48. 962 47. 535 47. 084 47. 399 48. 341 48. 657 46. 775 47. 084	35. 765 36. 081 36. 407 35. 293 35. 462 34. 425	40. 487 40. 487 41. 903 42. 861 43. 872 44. 741 42. 741 43. 605	1.00 33.55 1.00 33.46 1.00 32.64 1.00 33.83 1.00 34.11 1.00 34.24 1.00 35.64	A A A A A A	N C C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	136 137 138 139 140 141 142	CZ OH C O N CA CB	TYR TYR TYR TYR ARG ARG ARG	53 53 53 53 54 54 54	48. 026 48. 343 47. 266 47. 486 46. 773 46. 526 46. 993	33. 199 32. 170 37. 248 38. 404 36. 929 37. 933 37. 387	44. 601 45. 453 39. 548 39. 895 38. 355 37. 327 35. 972	1.00 35.74 1.00 35.79 1.00 33.40 1.00 33.56 1.00 34.36 1.00 34.87 1.00 35.72	A A A A A A	C O C O N C C
ATOM ATOM ATOM ATOM	143 144 145 146	CG CD NE CZ	ARG ARG ARG ARG	54 54 54 54	46. 887 47. 675 47. 651 46. 587	38. 373 37. 880 38. 831 39. 068	34. 821 33. 613 32. 506 31. 744	1.00 39.96 1.00 43.22 1.00 46.70 1.00 49.10	A A A	C C N C

(Continued)

FIG. 4-4

100M	1.47	ATIT 1	ADC.	E /I	45. 451	38.416	31.968	1.00 49.25	Α	N
ATOM	147		ARG	54 54	46.657	39. 957	30.757	1.00 50.00	Ä	N
ATOM	148		ARG	54 54	45.100	38. 445	37. 202	1.00 33.84	Ä	Ċ
ATOM	149		ARG		43. 100	37.687	37. 314	1.00 34.59	Ä	Ö
ATOM	150		ARG	54 55	44. 141	39. 748	36.966	1.00 33.05	Ä	Ň
ATOM	151		LEU	55		40. 402	36. 788	1.00 33.00	A	Ċ
ATOM	152		LEU	55	43.693	40. 402	37. 123	1.00 32.40	Ä	č
ATOM	153		LEU	55 55	43. 792	41. 694	38.557	1.00 23.14	Ä	Č
ATOM	154		LEU	55	44.042	43.847	38. 571	1.00 32.20	Ä	č
ATOM	155		LEU	55	44. 245	41.967	39. 448	1.00 31.66	A	č
ATOM	156	CD2		55	42.857	40. 271	35. 322	1.00 33.00	A	č
ATOM	157	-	LEU	55	43. 298	40. 769	34. 441	1.00 32.01	A	ŏ
ATOM	158	-	LEU	55 56	44.004	39. 593	35.050	1.00 33.02	Ä	Ň
ATOM	159		LYS	56 56	42.189	39. 462	33.673	1.00 31.32	A	Ċ
ATOM	160		LYS	56 56	41.733	38. 453	33. 564	1.00 31.42	A	Č
ATOM	161		LYS	56	40.584	36. 4 33	33. 733	1.00 34.84	Ä	Č
ATOM	162		LYS	56 56	40.978	36. 484	32. 530	1.00 34.84	A	Č
ATOM	163		LYS	56 56	41.746	35. 009	32. 698	1.00 40.95	A	č
ATOM	164		LYS	56 56	42.120 43.117	34. 537	31.685	1.00 43.33	A	N
ATOM	165	NZ	LYS	56 56	41. 240	40. 844	33. 252	1.00 30.03	A	Ċ
ATOM	166	C	LYS	56	40.839	40. 644	34. 088	1.00 28.24	A	ŏ
ATOM	167	0	LYS	56 57	40. 835	41. 120	31.956	1.00 20.24	A	N
ATOM	168		LEU	57	40.836	42. 404	31. 437	1.00 30.20	A	C
ATOM	169		LEU	57	40. 030	43. 233	30. 934	1.00 25.45	A	č
ATOM	170	CB	LEU	57	43. 230	43. 474	31.844	1.00 32.13	Ä	č
ATOM	171	CG	LEU	57	43. 230	43. 414	31. 194	1.00 32.13	A	Č
ATOM	172	CD1		57	44. 123	43. 949	33. 230	1.00 25.00	A	č
ATOM	173	CD2 C	LEU	57	39. 911	43. 343	30. 271	1.00 28.16	A	č
ATOM	174		LEU	57	39. 668	40. 980	29. 914	1.00 28.60	Ä	ŏ
ATOM	175	0 N		58	39. 394	43. 196	29. 676	1.00 26.69	, A	N
ATOM	176	N CA	TYR TYR	58	38. 530	43. 150	28. 518	1.00 25.82	A	Ċ
ATOM	177 178	CB	TYR	58	37. 071	42. 890	28. 934	1.00 25.51	Ä	č
ATOM	179	CG	TYR	58	36. 195	42. 420	27. 797	1.00 26.86	Ä	č
ATOM	180	CD1	TYR	58	36. 051	41.062	27. 514	1.00 26.92	Ä	č
ATOM ATOM	181	CE1	TYR	58	35. 294	40.631	26. 429	1.00 26.28	A	Č
ATOM	182		TYR	58	35. 557	43. 333	26. 965	1.00 25.26	Ä	Č
ATOM	183		TYR	58	34. 803	42. 911	25. 882	1.00 26.13	Ä	Č
ATOM	184	CZ	TYR	58	34. 675	41. 564	25. 619	1.00 25.74	A	Č
ATOM	185	OH	TYR	58	33. 928	41.160	24. 541	1.00 27.32	Ä	Ö
ATOM	186	C	TYR	58	38. 681	44. 288	27. 647	1.00 24.95	A	Č
ATOM	187	Ö	TYR	58	37. 837	45. 176	27. 680	1.00 24.68	A	0
ATOM	188	N	SER	59	39. 763	44. 338	26.876	1.00 24.05	Ä	Ň
ATOM	189	CA	SER	59	40. 037	45. 470	25. 997	1.00 24.31	Ā	Ĉ
	190	CB	SER	59	41.547	45. 657	25.817	1.00 24.38	A	Č
ATOM ATOM	191	OG	SER	59	42. 187	45. 931	27. 051	1.00 28.99	Ä	Ŏ
ATOM	192	C	SER	59	39. 405	45. 294	24. 628	1.00 23.54	Ä	Č
ATOM	193	0	SER	59	39. 795	44. 420	23. 860	1.00 24.84	Ā	Ŏ
ATOM	194	N	LEU	60	38. 430	46. 135	24. 319	1.00 23.51	Ä	Ñ.
ATOM	195	CA	LEU	60	37. 765	46.073	23. 031	1.00 22.96	Α	C
VION	100	Off	טטע	00	311100	10.010	20.001			-

					ाम	G. 4	- 5			(Continued)
ATOM	196	СВ	LEU	60	36. 256	45.910	23. 228	1.00 21.27	A	С
ATOM			LEU	60	35.528	46.977	24.048	1.00 20.80	Α	C
ATOM	198	CD1	LEU	60	35.373	48.227	23. 208	1.00 19.95	Α	C
ATOM		CD2		60	34. 159	46.466	24.488	1.00 18.91	Α	C
ATOM			LEU	60	38. 072	47.356	22. 279	1.00 23.42	A	C
ATOM			LEU	60	38. 507	48. 340	22.869	1.00 23.10	A	0
ATOM			ARG	61	37.862	47. 339	20. 971	1.00 25.94	A	N
ATOM			ARG	61	38. 102	48. 522	20. 153	1.00 27.08	A	C
ATOM			ARG	61	39. 364	48. 323	19. 299	1.00 29.17	A	C
ATOM			ARG	61	40.545	47.713	20.076	1.00 34.91	A	C
ATOM			ARG	61	41.790	48.612	20. 088 18. 772	1.00 38.62 1.00 41.15	A	C
ATOM			ARG ARG	61	42. 423 43. 337	48. 715 47. 871	18. 299	1.00 41.13	A A	N C
ATOM ATOM		CZ NH1		61 61	43. 754	46.848	19. 033	1.00 41.78	A	N N
ATOM		NH2		61	43. 821	48.042	17.076	1.00 43.39	A	N
ATOM			ARG	61	36.869	48. 724	19. 270	1.00 45.05	A	Č
ATOM		0	ARG	61	36.616	47. 939	18. 358	1.00 26.31	A	ő
ATOM		N	TRP	62	36. 087	49. 758	19.568	1.00 24.63	A	N
ATOM		CA	TRP	62	34. 883	50.050	18. 794	1.00 24.74	A	Ĉ
ATOM		CB	TRP	$6\overline{2}$	34. 092	51.207	19.420	1.00 23.22	Ā	Č
ATOM		ĊĞ	TRP	62	33. 472	50.900	20.741	1.00 23.78	Α	Ċ
ATOM		CD2		62	32.302	50.110	20.972	1.00 23.80	Α	C
ATOM	218	CE2	TRP	62	32.082	50.085	22.368	1.00 23.69	Α	C
ATOM		CE3		62	31.416	49.419	20.133	1.00 22.71	Α	С
ATOM		CD1		62	33.906	51.310	21.972	1.00 24.25	Α	С
ATOM		NE1		62	33. 075	50.824	22.955	1.00 23.12	A	N
ATOM		CZ2		62	31.013	49. 396	22. 945	1.00 23.91	A	C
ATOM		CZ3		62	30. 357	48. 736	20. 703	1.00 24.08	A	C
ATOM		CH2		62	30. 162	48. 730	22.100	1. 00 25. 02	A	C
ATOM		C	TRP	62	35. 241	50.427	17. 365	1.00 25.48	A	C
ATOM		0	TRP	62	35. 980	51.380	17. 138	1.00 27.15	A	0
ATOM		N	ILE	63	34. 722	49.682	16.398	1.00 26.16	A	N
ATOM		CA	ILE	63	35. 000 35. 312	49. 991 48. 727	15.003 14.180	1.00 25.88 1.00 25.95	A A	C C
ATOM ATOM		CB CG2		63 63	36. 494	48. 000	14. 783	1.00 25.35	A	Č
ATOM		CG2		63	34. 092	47.810	14. 138	1.00 24.70	A	Č
ATOM		CD1		63	34. 246	46.666	13. 174	1.00 25.35	A	č
ATOM		CDI	ILE	63	33. 788	50.680	14. 400	1.00 26.00	A	Č
ATOM		Õ	ILE	63	33. 803	51.075	13. 239	1.00 26.14	Ä	ŏ
ATOM		Ň	SER	64	32. 738	50.812	15. 202	1.00 26.48	A	Ň
ATOM		CA	SER	64	31.510	51.470	14.768	1.00 28.43	A	Ċ
ATOM		CB	SER	64	30. 764	50.603	13-754	1.00 27.24	A	Č
ATOM		0G	SER	64	30. 181	49. 481	14. 392	1.00 28.00	Α	0
ATOM		C	SER	64	30. 597	51.727	15.964	1.00 29.08	Α	C
ATOM		0	SER	64	31.008	51.606	17.119	1.00 26.71	Α	0
ATOM		N	ASP	65	29. 348	52.067	15.678	1.00 31.29	Α	N
ATOM		CA	ASP	65	28.382	52.336	16.732	1.00 34.90	Α	С
ATOM			ASP	65	27. 384	53. 397	16. 269	1.00 37.81	A	C
ATOM	244	CG	ASP	65	26. 515	53. 905	17. 395	1.00 41.52	Α	С

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								(Continued)
				FIG	. 4 - 6			•
ATOM	245	OD1 ASP	65	27.070 54	. 235 18. 465	1.00 43.44	A	0
ATOM	246	OD2 ASP	65		. 986 17. 211	1.00 44.76	A	0
ATOM	247	C ASP	65		. 064 17. 128	1.00 34.55	A	С
ATOM	248	0 ASP	65		. 091 17. 981	1.00 33.76	Α	0
ATOM	249	N HIS	66		. 946 16. 520	1.00 34.31	Α	N
ATOM	250	CA HIS	66		. 679 16. 807	1.00 35.30	A	C
ATOM	251	CB HIS	66	26.555 48	. 229 15. 589	1.00 37.74	A	C
ATOM	252	CG HIS	66	25.648 49	. 288 15. 052	1.00 42.72	Α	C
ATOM	253	CD2 HIS	66		. 393 15. 056	1.00 44.80	A	C
ATOM	254	ND1 HIS	66		. 438 14. 455	1.00 45.16	A	Ņ
ATOM	255	CE1 HIS	66		. 206 14. 114	1.00 46.24	A	C
ATOM	256	NE2 HIS	66		. 595 14. 468	1.00 46.79	A	N
ATOM	257	C HIS	66		. 555 17. 223	1.00 33.78	A	C
ATOM	258	0 HIS	66		. 736 18. 068	1.00 34.67	A	0
ATOM	259	N GLU	67		. 501 16. 635	1.00 31.93	A	N
ATOM	260	CA GLU	67		. 434 16. 979	1.00 31.45	A	C
ATOM	261	CB GLU	67		. 463 15. 801	1.00 31.46	A	C C
ATOM	262	CG GLU	67		. 103 14. 447	1.00 33.17	Α Α	C
ATOM	263	CD GLU	67 67		.092 13.311	1.00 35.48	A	C
ATOM	264	OE1 GLU	67 67		.090 13.394	1.00 32.44	A	0
ATOM	265	OE2 GLU	67		. 306 12. 329 . 866 17. 442	1.00 36.60 1.00 29.97	A A	C 0
ATOM	266	C GLU	67		. 866 17. 442 . 003 17. 241	1.00 29.91	A	0
ATOM ATOM	$\begin{array}{c} 267 \\ 268 \end{array}$	O GLU N TYR	.67 68		. 940 18. 088	1.00 30.44	A	N N
ATOM	269	CA TYR	68		. 190 18. 567	1.00 28.87	A	Ċ
ATOM	270	CR TYR	68		. 447 20. 073	1.00 26.31	A	č
ATOM	271	CG TYR	68		.324 20.917	1.00 23.19	Ä	č
ATOM	272	CD1 TYR	68		376 21.400	1.00 21.93	Ä	Č
ATOM	273	CE1 TYR	68		. 372 22. 231	1.00 21.10	A	Č
ATOM	274	CD2 TYR	68		. 232 21. 281	1.00 23.23	Α	C
ATOM .	275	CE2 TYR	68		225 22.110	1.00 22.67	Α	C
ATOM	276	CZ TYR	68		3.305 22.582	1.00 22.02	Α	C
ATOM	277	OH TYR	68		23. 403	1.00 22.72	Α	0
ATOM	278	C TYR	68	34.747 44	. 987 18. 256	1.00 29.51	Α	C
ATOM	279	0 TYR	68		3. 885 18. 028	1.00 28.32	A	0
ATOM	280	n leu	69		5. 202 18. 233	1.00 29.87	A	N
ATOM	281	CA LEU	69		. 115 17. 963	1.00 32.20	A	Č
ATOM	282	CB LEU	69		. 602 17. 106	1.00 30.73	A	C
ATOM	283	CG LEU	69		0.065 15.700	1.00 30.62	A	C
ATOM	284	CD1 LEU	69		6.629 14.963	1.00 29.98	A	C
ATOM	285	CD2 LEU	69		3. 891 14. 943	1.00 30.17	A	C
ATOM	286	C LEU	69		3.588 19.292	1.00 34.73	A	C
ATOM	287	0 LEU	69		1.305 20.294	1.00 34.80	A	0 N
ATOM	288	N TYR	70 70		2. 334 19. 305 . 726 20. 528	1.00 37.39 1.00 42.16	A A	N C
ATOM	289	CA TYR	70 70		. 726 20. 528 . 359 21. 444	1.00 42.16	A	C
ATOM	290	CB TYR	70 70		0. 866 22. 799	1.00 42.00	A	C
ATOM	291	CG TYR CD1 TYR	70 70		697 23.657	1.00 43.00	. A	Č
ATOM ATOM	292 293	CE1 TYR	70		253 24.892	1.00 44.69	A	Č
VION	439	CDITIN	10	00.001 41	יידע טטע.	1.00 11.00	- 1	v

			FIG. 4-7	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	294 CD2 TYR 295 CE2 TYR 296 CZ TYR 297 OH TYR 298 C TYR 299 O TYR 300 N LYS 301 CA LYS	70 70 70 70 70 70 71 71	37. 421 39. 563 23. 213 1. 00 43. 93 37. 853 39. 104 24. 452 1. 00 44. 83 38. 563 39. 959 25. 286 1. 00 45. 17 39. 004 39. 532 26. 516 1. 00 47. 21 39. 249 40. 480 20. 240 1. 00 45. 46 38. 976 39. 752 19. 287 1. 00 46. 31 40. 254 40. 231 21. 072 1. 00 49. 93	A C A C A C A O A C A O A N A C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	302 CB LYS 303 CG LYS 304 CD LYS 305 CE LYS 306 NZ LYS 307 C LYS 308 O LYS 309 N GLN	71 71 71 71 71 71 71 71	42. 580 39. 460 21. 054 1. 00 54. 14 43. 075 40. 455 20. 031 1. 00 56. 37 44. 559 40. 712 20. 226 1. 00 58. 61 45. 126 41. 628 19. 159 1. 00 58. 78 46. 590 41. 830 19. 361 1. 00 60. 82 40. 790 37. 952 21. 889 1. 00 57. 38 41. 109 38. 062 23. 075 1. 00 58. 38 40. 158 36. 884 21. 406 1. 00 60. 30	A C A C A C A N A C A N N
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	310 CA GLN 311 CB GLN 312 CG GLN 313 CD GLN 314 OE1 GLN 315 NE2 GLN 316 C GLN 317 O GLN 318 N GLU	72 72 72 72 72 72 72 72 73	39. 816 35. 750 22. 261 1. 00 63. 23 38. 902 34. 775 21. 526 1. 00 64. 07 38. 313 33. 695 22. 417 1. 00 65. 84 37. 270 34. 240 23. 375 1. 00 66. 33 36. 251 34. 790 22. 952 1. 00 67. 19 37. 519 34. 092 24. 671 1. 00 66. 80 41. 122 35. 049 22. 607 1. 00 65. 34 41. 563 35. 058 23. 760 1. 00 67. 00 41. 736 34. 442 21. 597 1. 00 66. 09	A C A C A C A C A C A C A C A C A C A C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	319 CA GLU 320 CB GLU 321 CG GLU 322 CD GLU 323 OE1 GLU 324 OE2 GLU 325 C GLU 326 O GLU	73 73 73 73 73 73 73 73 73	43. 012 33. 763 21. 775 1. 00 67. 12 43. 008 32. 420 21. 046 1. 00 68. 53 41. 974 31. 433 21. 570 1. 00 71. 35 42. 223 31. 026 23. 012 1. 00 72. 71 41. 491 30. 147 23. 517 1. 00 73. 51 43. 147 31. 585 23. 643 1. 00 74. 16 44. 076 34. 681 21. 184 1. 00 66. 83 44. 563 35. 592 21. 857 1. 00 67. 65	A C A C A C A C A C A O A O A O
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	327 N ASN 328 CA ASN 329 CB ASN 330 CG ASN 331 OD1 ASN 332 ND2 ASN 333 C ASN 334 O ASN	74 74 74 74 74 74 74 74	44. 430 34. 442 19. 924 1. 00 65. 38 45. 411 35. 273 19. 236 1. 00 63. 38 46. 661 34. 466 18. 889 1. 00 64. 38 47. 654 34. 422 20. 034 1. 00 66. 10 48. 128 35. 463 20. 496 1. 00 65. 51 47. 973 33. 216 20. 503 1. 00 66. 62 44. 794 35. 859 17. 977 1. 00 61. 55 45. 384 36. 714 17. 318 1. 00 62. 15	A N A C A C A C A O A N A C A O
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	335 N ASN 336 CA ASN 337 CB ASN 338 CG ASN 339 OD1 ASN 340 ND2 ASN 341 C ASN 342 O ASN	75 75 75 75 75 75 75 75	43. 597 35. 390 17. 647 1. 00 58. 67 42. 888 35. 886 16. 481 1. 00 55. 82 42. 023 34. 785 15. 871 1. 00 57. 81 41. 410 33. 887 16. 916 1. 00 58. 63 40. 857 34. 358 17. 909 1. 00 59. 69 41. 500 32. 580 16. 697 1. 00 58. 92 42. 017 37. 045 16. 918 1. 00 52. 82 41. 630 37. 135 18. 081 1. 00 53. 60	A N A C A C A N A C A C A O A N A C A O

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(Continued) FIG. 4-8 15.985 1.00 49.11 A N 37. 937 41.715 76 ATOM 343 N ILE 1.00 44.67 C 39.091 16.294 A 40.893 ILE 76 344 CA ATOM 1.00 44.26 C 15.502 A 41.343 40.317 ILE 76 ATOM 345 CB C 1.00 43.37 41.533 15.956 A 40.565 346 CG2 ILE 76 ATOM 1.00 45.27 C A 42.841 40.547 15.716 CG1 ILE 76 ATOM 347 C 41.647 14.844 1.00 45.53 A 43.435 348 CD1 ILE 76 ATOM 1.00 42.80 C 15.964 Α 38.786 39.446 **ATOM** 349 C ILE 76 1.00 41.85 A 0 14.868 38. 322 350 0 ILE 76 39.127 **ATOM** 38.574 39.045 16.930 1.00 40.36 Α N LEU 77 351 N ATOM 16.772 1.00 37.65 A C 37.151 38.801 LEU 77 CA 352 **ATOM** C 37.948 17.933 1.00 36.65 A 36.636 CB LEU 77 **ATOM** 353 1.00 35.22 A C 18.264 37.363 36.642 354 LEU 77 ATOM CG C 1.00 34.43 Α 36.600 35.926 19.361 ATOM 355 CD1 LEU 77 C 1.00 34.38 Α 17.039 ATOM CD2 LEU 77 37.459 35.756 356 C 1.00 35.91 36.365 40.107 16.730 Α C LEU 77 **ATOM** 357 A 0 36.801 41.123 17.269 1.00 35.03 0 LEU 77 358 **ATOM** 40.069 16.070 1.00 34.19 A N 35.212 78 N VAL **ATOM** 359 1.00 31.96 C 34.330 41.226 15.981 Α 78 ATOM 360 CA VAL C 1.00 31.90 A 41.628 14.509 ATOM 361 CB VAL 78 34.078 C 1.00 31.34 362 CG1 VAL 78 33.612 40.420 13.704 Α ATOM C 33.048 42.747 14.442 1.00 31.56 A CG2 VAL 78 363 ATOM C 40.838 16.667 1.00 31.15 Α 33.011 78 364 C VAL **ATOM** Α 0 39.819 16.336 1.00 30.46 32.404 0 VAL 78 ATOM 365 1.00 29.90 N 32.582 41.643 17.636 Α N 79 **ATOM** 366 PHE 41.357 18.379 1.00 28.93 C 31.358 Α **ATOM** 367 CA PHE 79 C 1.00 29.14 PHE 79 31.618 41.420 19.888 A 368 CB ATOM C 1.00 28.39 32.357 40.238 20.440 A CG PHE 79 **ATOM** 369 C 33.704 40.051 20.165 1.00 28.20 A CD1 PHE 79 **ATOM** 370 31.701 1.00 27.22 C 39.314 21.243 A CD2 PHE **ATOM** 371 79 Č 38.956 20.684 1.00 28.13 A 34.391 372 CE1 PHE 79 **ATOM** C 38.219 1.00 27.53 A ATOM 373 CE2 PHE 79 32.374 21.764 Č CZ PHE 79 33.725 38.040 21.483 1.00 27.59 A 374 ATOM 1.00 29.06 C 30.186 42.281 18.091 A 79 ATOM 375 C PHE 17.912 1.00 28.29 0 30.354 43.487 A 0 PHE 79 ATOM 376 N A 41.704 18.058 1.00 27.80 ASN 28.990 **ATOM** 377 N 80 C 27.791 42.499 17.864 1.00 27.95 Α 378 CA ASN **ATOM** 80 1.00 27.03 C 41.670 17.209 26.681 Α 379 CB ASN 80 ATOM 1.00 27.26 C 42.412 17.160 A CG ASN 25.354 380 80 **ATOM** 18.182 1.00 26.87 Α 0 24.679 42.587 381 OD1 ASN 80 **ATOM** 15.974 24.980 42.866 1.00 26.94 A N ND2 ASN **ATOM** 382 80 1.00 28.06 19.289 C 27.405 42.874 Α C ASN 80 **ATOM** 383 20.066 1.00 28.61 Α 0 26.991 42.024 **ATOM** 384 0 ASN 80 27.566 44.140 19.642 1.00 28.12 Α N N ALA 81 **ATOM** 385 20.991 1.00 29.16 C

SUBSTITUTE SHEET (RULE 26)

44.579

46.075

44.254

43.769

44.506

44. 282

21.119

21.413

22.527

20.516

20.809

Α

Α

A

Α

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C

C

0

N

C

1.00 27.93

1.00 31.04

1.00 30.16

1.00 32.39

1.00 34.46

27.250

27.503

25.818

25.582

24.870

23.461

CA

CB

0

N

CA

386

387

388 C

389

390

391

ATOM

ATOM

ATOM

ATOM

ATOM

ATOM

ALA

ALA

ALA

ALA

GLU

GLU

81

81

81

81

82

82

										(Continued)
					FΙ	G. 4	- 9			•
ATOM	392	СВ	GLU	82	22.602	44. 794	19.655	1.00 36.97	A	С
ATOM	393	CG	GLU	82 82	21.115	44. 827	19.968	1.00 40.49	Ä	č
ATOM ATOM	394	CD	GLU	82 82	20. 313	45. 538	18.894	1.00 44.05	A	č
ATOM	395		GLU	82	20. 343	45.087	17. 726	1.00 45.13	A	ő
ATOM	396	0E2		82	19.652	46.551	19. 220	1.00 45.61	A	Ö
ATOM	397	C	GLU	82	23.042	42.853	21.153	1.00 33.95	A	Č
ATOM	398	Ö	GLU	82	22.055	42.662	21.864	1.00 32.29	A	Ö
ATOM	399	N	TYR	83	23. 777	41.857	20.666	1. 00 33. 23	A	N
ATOM	400	CA	TYR	83	23. 423	40.468	20.947	1.00 33.39	Ā	Ċ
ATOM	401	CB	TYR	83	22. 846	39.810	19.686	1.00 34.54	A	С
ATOM	402	CG	TYR	83	21.690	40.594	19.109	1.00 34.80	Α	C
ATOM	403	CD1	TYR	83	20. 558	40.859	19.878	1.00 35.22	A	C
ATOM	404	CE1	TYR	83	19. 527	41.657	19.396	1.00 36.27	A	C
ATOM	405		TYR	83	21.759	41.139	17.828	1.00 35.71	Α	С
ATOM	406		TYR	83	20.731	41.940	17.331	1.00 37.42	Α	C
ATOM	407	CZ	TYR	83	19.619	42.200	18.125	1.00 37.70	Α	C
ATOM	408	OH	TYR	83	18.624	43.044	17.675	1.00 37.69	Α	0
ATOM	409	C	TYR	83	24.582	39.644	21.494	1.00 33.19	Α	C
ATOM	410	0	TYR	83	24.396	38.511	21.934	1.00 32.91	Α	0
ATOM	411	N	GLY	84	25.777	40.217	21.476	1.00 33.53	Α	N
ATOM	412	CA	GLY	84	26.933	39.513	21.995	1.00 33.40	Α	С
ATOM	413	C	GLY	84	27.454	38.395	21.114	1.00 33.92	Α	C
ATOM	414	0	GLY	84	28. 329	37.639	21.530	1.00 33.21	Α	0
ATOM	415	N	ASN	85	26.918	38.269	19.904	1.00 35.26	Α	N
ATOM	416	CA	ASN	85	27. 388	37.233	18.993	1.00 37.43	Α	С
ATOM	417	CB	ASN	85	26.258	36.780	18.072	1.00 38.34	Α	C
ATOM	418	CG	ASN	85	25.764	37.878	17.166	1.00 40.02	Α	C .
ATOM	419	0D1	ASN	85	25.694	39.040	17.561	1.00 39.96	Α	0
ATOM	420	ND2	ASN	85	25.394	37.496	15.950	1.00 41.91	A	N
ATOM	421	C	ASN	85	28.556	37. 794	18. 188	1.00 38.80	A	C
ATOM	422	0	ASN	85	28.687	39.011	18.035	1.00 40.05	Α	0
ATOM	423	N	SER	86	29.410	36.920	17.670	1.00 39.14	A	N
ATOM	424	CA	SER	86	30. 565		16.926	1.00 39.30	A	C
ATOM	425	CB	SER	86	31.723		17.895	1.00 38.90	A	C
ATOM	426	0G	SER	86	32.041	36.356	18. 515	1.00 35.77	A	0
ATOM	427	C	SER	86	31.023	36. 482	15. 798	1.00 39.94	A	C
ATOM	428	0	SER	86	30. 287	35.622	15. 323	1.00 41.15	A	0
ATOM	429	N	SER	87	32. 264	36.701	15. 382	1.00 40.59	A	N
ATOM	430	CA	SER	87	32.916	35. 929	14. 333	1.00 40.98	A	C
ATOM	431	CB	SER	87	32. 152	36.053	13.010	1.00 39.16	A	C
ATOM	432	0G	SER	87	31.727	37. 376	12.789	1.00 39.90	A	0
ATOM	433	C	SER	87	34. 353	36. 433	14. 194	1.00 41.10	A	C
ATOM	434	0	SER	87	34. 691	37.517	14.682	1.00 41.07	A	0
ATOM	435	N	VAL	88	35. 206	35. 646	13.548	1.00 41.07	A	N
ATOM	436	CA	VAL	88	36. 596	36.043	13.402	1.00 41.43	A	C
ATOM	437	CB	VAL	88	37. 502	34. 836	13.114	1.00 41.29	A	C
ATOM	438		VAL	88	38. 949	35. 295	13.013	1.00 41.30	A	C
ATOM	439		VAL	88	37. 361	33.808	14. 222	1.00 40.28	A	C C
ATOM	440	C	VAL	88	36. 827	37.096	12. 331	1.00 41.63	A	U

					FIG	G. 4-	10			(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	441 442 443 444 445 445 451 453 454 455 457 458 466 467 467 473 475 476 477 478	N CA CB CG CD1 CE2 CZ C O N CA CB CG CD1 CE2 CZ C O N CA CB CG CD1 CE2 C O N CA CB CG CD1 ND2 C O N CA CB CG CD1 ND2 C O	PHE PHE PHE LEU LEU LEU GLU GLU GLU ASN ASN ASN ASN ASN ASN ASN	88 89 89 89 89 89 89 89 89 90 90 90 90 91 91 91 91 91 91 92 92 92 92 92 92 92 92 93 93 93 94 95 96 97 97 98 99 90 90 90 90 90 90 90 90 90	F I 6 36. 548 37. 343 37. 641 37. 769 37. 990 39. 217 36. 963 39. 415 37. 154 38. 381 38. 956 39. 851 41. 143 42. 071 43. 033 42. 236 43. 933 41. 718 42. 063 41. 815 42. 335 41. 817 42. 048 41. 454 41. 875 40. 566 43. 855 44. 572 44. 322 45. 738 45. 189 44. 420 46. 622 47. 806 46. 059	36. 885 38. 238 39. 347 40. 637 41. 865 42. 778 43. 231 43. 911 44. 135 39. 021 39. 335 38. 001 39. 213 39. 305 39. 408 40. 515 36. 907 37. 159 35. 694 34. 559 33. 243 33. 070 31. 774 30. 694 31. 833 34. 521 34. 841 34. 117 34. 028 33. 389 32. 082 31. 248 31. 894 33. 061	1 0 11. 154 12. 767 11. 880 12. 699 11. 870 11. 265 11. 678 10. 894 10. 295 11. 186 10. 019 11. 921 11. 380 11. 366 10. 184 8. 889 10. 346 12. 267 13. 421 11. 726 12. 482 11. 891 10. 403 9. 879 10. 350 9. 001 12. 588 11. 641 13. 766 14. 100 15. 477 15. 585 14. 684 16. 691 13. 111 13. 370 11. 984	1. 00 41. 38 1. 00 42. 23 1. 00 42. 51 1. 00 40. 84 1. 00 39. 96 1. 00 39. 62 1. 00 40. 08 1. 00 39. 60 1. 00 39. 50 1. 00 43. 57 1. 00 43. 57 1. 00 45. 92 1. 00 48. 60 1. 00 48. 66 1. 00 49. 47 1. 00 50. 17 1. 00 50. 17 1. 00 50. 91 1. 00 53. 65 1. 00 50. 91 1. 00 53. 65 1. 00 60. 92 1. 00 62. 39 1. 00 63. 50 1. 00 56. 93 1. 00 56. 93 1. 00 57. 64 1. 00 59. 59 1. 00 59. 59	A A A A A A A A A A A A A A A A A A A	
ATOM ATOM ATOM	478 479	O N CA	SER SER	93 93	46. 059 46. 828	32. 862 32. 127	11.984 10.991	1.00 60.45 1.00 61.76	A A	N C
ATOM ATOM ATOM ATOM ATOM ATOM	480 481 482 483 484 485	CB OG C O N CA	SER SER SER SER THR THR	93 93 93 93 94 94	45. 978 46. 714 47. 296 48. 314 46. 552 46. 852	30. 985 30. 198 33. 030 32. 765 34. 103 35. 036	10. 427 9. 507 9. 853 9. 213 9. 618 8. 541	1.00 62.43 1.00 64.10 1.00 62.23 1.00 62.82 1.00 62.37 1.00 62.69	A A A A A	C O C O N C
ATOM ATOM ATOM ATOM	486 487 488 489	CB OG1 CG2	THR	94 94 94 94	45. 982 46. 469 46. 003 48. 306	36. 298 37. 302 36. 821	8. 659 7. 759 10. 080 8. 377	1.00 63.25 1.00 63.59 1.00 64.14 1.00 62.28	A A A	C 0 C C

										(Continued)
					FIG	G. 4	- 11			
ATOM	490	0	THR	94	48.882	35. 295	7. 303	1.00 61.92	A	0
ATOM	491	Ň	PHE	95	48.908	36.013	9.426	1.00 62.57	Α	N
ATOM	492	CA	PHE	95	50. 290	36.473	9.322	1.00 63.04	Α	C
ATOM	493	CB	PHE	95	50.414	37.889	9.897	1.00 61.98	Α	C
ATOM	494	ĊĠ	PHE	95	49.456	38.869	9.289	1.00 61.01	Α	C
ATOM	495	CD1		95	48. 248	39.155	9.911	1.00 60.97	Α	C
ATOM	496	CD2		95	49.742	39.473	8.073	1.00 60.73	Α	C
ATOM	497	CE1		95	47.337	40.026	9.330	1.00 60.46	Α	C .
ATOM	498	CE2		95	48.838	40.343	7.483	1.00 60.09	Α	C ·
ATOM	499	CZ	PHE	95	47.633	40.621	8.113	1.00 61.07	Α	C
ATOM	500	Ċ	PHE	95	51.346	35.571	9.956	1.00 63.20	Α	C
ATOM	501	0	PHE	95	52.178	36.035	10.736	1.00 63.66	Α	0
ATOM	502	N	ASP	96	51.323	34. 288	9.611	1.00 63.37	Α	. N
ATOM	503	CA	ASP	96	52.298	33. 347	10.149	1.00 64.05	Α	C
ATOM	504	CB	ASP	96	51.771	31.913	10.044	1.00 65.11	A	C
ATOM	505	CG	ASP	96	50.747	31.589	11.115	1.00 65.73	Α	C
ATOM	506	0D1	ASP	96	49.758	32.342	11.240	1.00 66.41	Α	0
ATOM	507	0D2	ASP	96	50.929	30.580	11.829	1.00 65.32	Α	0
ATOM	508	C	ASP	96	53.621	33.470	9.399	1.00 63.82	Α	C
ATOM	509	0	ASP	96	54.696	33. 433	10.001	1.00 64.05	A	0
ATOM	510	N	GLU	97	53.540	33.619	8.083	1.00 62.95	Α	N
ATOM	511	CA	GLU	97	54.740	33.754	7. 271	1.00 62.73	Α	C
ATOM	512	CB	GLU	97	54.596	32.964	5.965	1.00 65.91	A	С
ATOM	513	CG	GLU	97	54.954	31.478	6.064	1.00 68.84	Α	C
ATOM	514	CD	GLU	97	53.945	30.657	6.850	1.00 70.64	Α	C
ATOM	515	0E1	GLU	97	54.160	29.432	6.988	1.00 71.38	Α	0
ATOM	516	0E2		97	52.939	31.228	7.325	1.00 71.80	Α	0
ATOM	517	C	GLU	97	55.039	35.220	6.963	1.00 60.82	Α	C
ATOM	518	0	GLU	97	55.462	35.557	5.857	1.00 60.31	Α	0
ATOM	519	N	PHE	98	54.818	36.084	7. 952	1.00 58.68	Α	N
ATOM	520	CA	PHE	98	55.067	37.513	7.797	1.00 55.93	Α	C
ATOM	521	CB	PHE	98	54. 200	38.319	8.765	1.00 55.47	A	C
ATOM	522	CG	PHE	98	54.272	39.801	8. 542	1.00 54.84	Α	C
ATOM	523		PHE	98	53.712	40.372	7. 404	1.00 53.07	Α	C
ATOM	524	CD2		98	54. 931	40.624	9. 450	1.00 53.89	A	C
ATOM	525		PHE	98	53, 808	41.743	7. 173	1.00 53.28	A	С
ATOM	526		PHE	98	55.032	41.997	9. 226	1.00 53.18	A	C
ATOM	527	CZ	PHE	98	54. 470	42.556	8.087	1.00 52.22	Α	C
ATOM	528	C	PHE	98	56.536	37.820	8.060	1.00 54.61	Α	C
ATOM	529	0	PHE	98	57.041	38. 878	7. 686	1.00 53.80	Α	0
ATOM	530	N	GLY	99	57. 215	36.885	8. 713	1.00 53.53	Α	N
ATOM	531	CA	GLY	99	58. 624	37.061	9.004	1.00 52.08	A	C
ATOM	532	C	GLY	99	58. 908	38. 188	9. 972	1.00 51.18	A	C
ATOM	533	0	GLY	99	60.037	38.673	10.051	1.00 51.30	Α	0
ATOM	534	N	HIS	100	57.884	38.607	10.706	1.00 50.21	Α	N
ATOM	535	CA	HIS	100	58.026	39. 681	11.686	1.00 49.15	Α	С
ATOM	536	CB	HIS	100	57.810	41.049	11.028	1.00 48.84	Α	C
ATOM	537		HIS	100	58.850	41.410	10.014	1.00 49.22	Α	C
ATOM	538	CD2	HIS	100	58. 759	41.613	8. 679	1.00 49.42	Α	С

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ATOM	539	ND1	HIS	100	60.170	41.627	10.346	1.00 49.70	Α	N
ATOM	540		HIS	100	60.848	41.951	9. 259	1.00 49.10	A	C
ATOM	541		HIS	100	60.015	41.949	8. 234	1.00 50.14	Ą	N
ATOM	542	С	HIS	100	57.011	39. 511	12.810	1.00 48.06	A	C
ATOM	543	0	HIS	100	55.920	38.977	12.602	1.00 47.18	A	0
ATOM	544	N	SER	101	57. 377	39.958	14.005	1.00 46.66	A	N
ATOM	545	CA	SER	101	56. 467	39. 878	15. 136	1.00 45.88	A	Ç
ATOM	546	CB	SER	101	57.247	39. 802	16.446	1.00 47.41	Α	C
ATOM	547	0G	SER	101	58.118	38.685	16.447	1.00 51.04	Α	0
ATOM	548	C	SER	101	55.617	41.142	15.112	1.00 44.53	A	C
ATOM	549	ŏ	SER	101	56.133	42. 248	15. 282	1.00 44.41	Ä	Ö
ATOM	550	N	ILE	102	54.319	40.976	14. 877	1.00 41.90	A	N
ATOM	551	CA	ILE	102	53. 409	42.109	14. 833	1.00 38.95	A	C
ATOM	552	CB	ILE	102	52.106	41.732	14. 117	1.00 38.54	A	C
ATOM	553	CG2	ILE	102	51.153	42.926	14. 103	1.00 38.18	A	Č
ATOM	554	CG1	ILE	102	52. 424	41. 288	12.686	1.00 37.65	A	č
ATOM	555	CD1	ILE	102	51. 243	40. 733	11. 937	1.00 37.11	A	C
ATOM	556	С	ILE	102	53. 104	42.597	16. 244	1.00 38.00	A	C
ATOM	557	0	ILE	102	52.441	41.919	17.024	1.00 38.06	Α	0
ATOM	558	N	ASN	103	53.601	43.787	16.556	1.00 37.54	Α	N
ATOM	559	CA	ASN	103	53. 429	44. 399	17. 867	1.00 36.65	Ä	Ċ
ATOM	560	CB	ASN	103	54. 437	45. 530	18. 039	1.00 37.69		Č
									A	
ATOM	561	CG	ASN	103	54. 219	46.308	19. 315	1.00 39.56	A	C
ATOM	562	0D1	ASN	103	54.655	45.891	20. 388	1.00 43.00	Α	0
ATOM	563	ND2	ASN	103	53. 528	47.439	19. 211	1.00 38.34	Α	N
ATOM	564	C	ASN	103	52.031	44.953	18.116	1.00 35.79	A	С
ATOM	565	0	ASN	103	51.532	44.910	19. 237	1.00 35.79	Ä	Ŏ
ATOM	566	Ň	ASP	104	51.405	45.490	17. 078	1.00 34.43		
									A	N
ATOM	567	CA	ASP	104	50.079	46.067	17. 236	1.00 33.27	A	C
ATOM	568	CB	ASP	104	50. 200	47. 388	17. 998	1.00 34.38	A	C
ATOM	569	CG	ASP	104	48.896	47.823	18.618	1.00 34.79	A	C
ATOM	570	0D1	ASP	104	48.916	48.699	19.509	1.00 33.92	Α	0
ATOM	571		ASP	104	47.852	47. 289	18. 207	1.00 36.80	A	Ŏ
ATOM	572	C	ASP	104	49. 436	46. 281	15. 865	1.00 32.32		
									A	C
ATOM	573	0	ASP	104	50.124	46.326	14.850	1.00 32.03	A	0
ATOM	574	N	TYR	105	48. 118	46. 405	15.834	1.00 31.15	Α	N
ATOM	575	CA	TYR	105	47. 421	46.580	14.570	1.00 32.24	Α	C
ATOM	576	CB	TYR	105	46.672	45.296	14. 223	1.00 34.70	A	C
ATOM	577	CG	TYR	105	45. 443	45.088	15. 072	1.00 37.73	Ä	č
ATOM	578		TYR	105	44. 220	45.636	14. 698	1.00 37.51		
									A	C
ATOM	579		TYR	105	43. 098	45. 510	15. 506	1.00 40.43	A	C
ATOM	580		TYR	105	45. 514	44. 395	16. 284	1.00 39.06	A	C
ATOM	581	CE2	TYR	105	44.393	44.263	17. 103	1.00 40.75	A	C
ATOM	582	CZ	TYR	105	43. 191	44.829	16.705	1.00 41.19	Α	C
ATOM	583	OH	TYR	105	42.088	44.755	17.519	1.00 44.27	Ä	Ŏ
ATOM	584	C	TYR	105	46. 441	47. 743	14. 638	1.00 31.43	A	Č
ATOM										
	585	0	TYR	105	46. 133	48. 249	15. 715	1.00 30.78	A	0
ATOM	586	N	SER	106	45. 940	48. 152	13. 479	1.00 30.16	A	N
ATOM	587	CA	SER	106	45. 000	49. 261	13.415	1.00 29.23	Α	C

			•					,		(Continued)
					ान	G. 4	- 13		•	(Continued)
						· ·				
ATOM	588	CB	SER	106	45.762		13.457	1.00 29.81	A	C
ATOM	589	0G	SER	106	44. 924		13.090	1.00 32.32	A	0
ATOM	590	C	SER	106	44. 146		12. 157	1.00 27.65	A	C
ATOM	591	0	SER	106	44. 657			1.00 28.57	A	0
ATOM	592	N	ILE	107	42. 835		12.331	1.00 28.07	A	N
ATOM	593	CA	ILE	107	41.922		11. 198 11. 544	1.00 27.70 1.00 25.83	A A	C C
ATOM ATOM	594 595	CB CG2	ILE	107 107	40. 648 39. 557		10. 522	1.00 25.85	A	C
ATOM	596	CG2		107	40. 970		11.551	1.00 25.36	A	Č
ATOM	597	CD1		107	41. 980		12.568	1.00 23.77	A	Č
ATOM	598	CD1	ILE	107	41.502		10. 743	1.00 26.85	A	č
ATOM	599	ő	ILE	107	41.178		11.557	1.00 26.55	A	Ö
ATOM	600	Ň	SER	108	41.507	50. 757	9. 432	1.00 27.57	A	N
ATOM	601		SER	108	41.113		8.862	1.00 26.94	Α	С
ATOM	602	CB	SER	108	41.331	52.033	7.346	1.00 26.30	Α	C.
ATOM	603	0G	SER	108	40.458		6.700	1.00 23.63	Α	0
ATOM	604	C	SER	108	39. 639		9. 169	1.00 27.22	Α	С
ATOM	605	0	SER	108	38. 857		9. 206	1.00 26.49	A	0
ATOM	606		PRO	109	39. 241		9. 393	1.00 28.50	A	N
ATOM	607		PRO	109	40. 025		9. 302	1.00 29.19	A	C
ATOM	608		PRO	109	37. 839		9.693	1.00 29.39	A	C
ATOM	609		PRO	109	37. 745		9.439	1.00 30.19	A	C C
ATOM ATOM	610 611		PRO PRO	109 109	39. 080 36. 842		9. 899 8. 852	1.00 28.76 1.00 29.21	·A A	C
ATOM	612		PRO	109	35. 901		9. 391	1.00 29.21	A	0
ATOM	613		ASP .	110	37. 046		7. 540	1.00 29.41	A	Ň
ATOM	614		ASP	110	36. 120		6.676	1.00 28.98	A	Ċ
ATOM	615	CB	ASP	110	36. 241		5. 226	1.00 27.99	A	Č
ATOM	616	CG	ASP	110	37.613		4.648	1.00 27.91	A	C
ATOM	617	0D1	ASP	110	38. 226		4. 976	1.00 28.41	A	0
ATOM	618	0D2		110	38.075		3.852	1.00 29.14	A	0
ATOM	619	C	ASP	110	36. 280		6.715	1.00 29.06	A	С
ATOM	620	0	ASP	110	35. 635		5. 953	1.00 30.84	A	0
ATOM	621	N	GLY	111	37. 148		7. 589	1.00 28.25	A	N
ATOM	622		GLY	111		48. 766	7. 702	1.00 28.14	A	C
ATOM	623		GLY	111	37.890		6.470	1.00 29.53	A	C
ATOM ATOM	624 625	O N	GLY GLN	111	37. 856		6. 402 5. 503	1.00 31.16 1.00 29.61	A A	O N
ATOM	626		GLN	112 112	38. 405 38. 946		4. 287	1.00 29.01	A	C
ATOM	627		GLN	112	38. 777		3. 109	1.00 29.94	A	č
ATOM	628		GLN	112	37. 336		2. 749	1.00 23.34	A	č
ATOM	629		GLN	112	37. 191		1.465	1.00 33.24	A	č
ATOM	630	0E1		112	36. 075		1.004	1.00 36.27	A	Ö ·
ATOM	631	NE2		112	38. 314		0. 880	1.00 31.73	A	Ň
ATOM	632	C	GLN	112	40. 415		4.390	1.00 30.31	A	C
ATOM	633		GLN	112	40.888		3. 631	1.00 31.75	Α	0
ATOM	634		PHE	113	41.141	48. 418	5. 320	1.00 29.82	Α	N
ATOM	635		PHE	113	42. 551		5. 486	1.00 28.23	A	C
ATOM	636	CB	PHE	113	43. 428	49. 207	4. 900	1.00 24.48	A	С

		·	F`I G. 4	- 14			(Continued)
ATOM	637 CG PHE	113	43.193 49.467	3.458	1.00 22.98	A	C
ATOM	638 CD1 PHE	113	42.164 50.301	3.052	1.00 20.83	A	C
ATOM	639 CD2 PHE	113	44.010 48.880	2.496	1.00 23.28	A	C
ATOM	640 CE1 PHE	113	41. 950 50. 552	1.709	1.00 20.79	A	C
ATOM	641 CE2 PHE	113	43. 805 49. 121	1.150	1.00 22.78	A	C
ATOM	642 CZ PHE	113	42.771 49.962	0.754	1.00 22.17	A	C
ATOM	643 C PHE	113	42.919 47.974	6.947	1.00 30.31 1.00 31.09	A	C 0
ATOM	644 0 PHE	113	42. 234 48. 511	7.827	1.00 31.09	A A	N ·
ATOM	645 N ILE	114	44. 013 47. 260 44. 521 47. 092	7. 196 8. 542	1.00 29.70	A	C
ATOM	646 CA ILE	114	44.342 45.642	9. 075	1.00 30.73	A	č
ATOM	647 CB ILE 648 CG2 ILE	114 114	44. 804 44. 633	8. 042	1.00 31.12	A	Č.
ATOM ATOM	648 CG2 ILE 649 CG1 ILE	114	45. 128 45. 475	10. 381	1.00 32.62	A	Č
ATOM	650 CD1 ILE	114	45. 028 44. 092	11.007	1.00 33.60	Ä	č
ATOM	651 C ILE	114	46.000 47.457	8. 509	1.00 30.59	Ä	Č
ATOM	652 0 ILE	114	46.754 46.974	7.661	1.00 28.76	Ā	0
ATOM	653 N LEU	115	46.388 48.343	9. 423	1.00 30.68	A	N
ATOM	654 CA LEU	115	47.759 48.814	9.543	1.00 29.92	Α	C
ATOM	655 CB LEU	115	47.769 50.257	10.053	1.00 30.35	Α	
ATOM	656 CG LEU	115	49. 135 50. 941	10.131	1.00 31.72	Α	C C C
ATOM	657 · CD1 LEU	115	49.668 51.147	8.718	1.00 33.17	Α	C
ATOM	658 CD2 LEU	115	49.018 52.271	10.857	1.00 30.77	A	C
ATOM	659 C LEU	115	48. 481 47. 911	10.530	1.00 29.61	A	C
ATOM	660 0 LEU	115	48.127 47.861	11.707	1.00 30.77	A	0 ·
ATOM	661 N LEU	116	49.484 47.188	10.048	1.00 28.74	A	N C
ATOM	662 CA LEU	116	50. 245 46. 278	10.891	1.00 28.06	A	C
ATOM	663 CB LEU	116	50. 624 45. 023 49. 450 44. 251	10. 103 9. 481	1.00 30.07 1.00 30.51	A A	r r
ATOM	664 CG LEU 665 CD1 LEU	116 116	49. 450 44. 251 49. 978 43. 171	8. 570	1.00 30.31	A	C C C C
ATOM ATOM	666 CD2 LEU	116	48. 583 43. 644	10. 573	1.00 30.99	A	r.
ATOM	667 C LEU	116	51.489 46.997	11. 363	1.00 28.28	A	Č
ATOM	668 0 LEU	116	52.145 47.690	10. 591	1.00 30.37	Ä	Ö
ATOM	669 N GLU	117	51.813 46.824	12.634	1.00 27.78	Ā	N
ATOM	670 CA GLU	117	52.962 47.484	13. 227	1.00 26.58	Α	C
ATOM	671 CB GLU	117	52.476 48.358	14.382	1.00 25.51	Α	С
ATOM	672 CG GLU	117	53.510 49.241	15.036	1.00 23.69	Α	C C
ATOM	673 CD GLU	117	52.897 50.076	16. 138	1.00 27.72	Α	C
ATOM	674 OE1 GLU	117	52.732 49.572	17. 268	1.00 29.08	A	0
ATOM	675 OE2 GLU	117	52. 552 51. 242	15.868	1.00 30.62	Ą	0
ATOM	676 C GLU	117	53. 997 46. 491	13. 738	1.00 27.81	A	C
ATOM	677 O GLU	117	53.666 45.586	14. 506	1.00 27.41	A	0
ATOM	678 N TYR	118	55. 247 46. 663	13. 313	1.00 27.75	A	N C
ATOM	679 CA TYR	118	56. 327 45. 796	13.765	1.00 29.68 1.00 29.52	A A	C C
ATOM	680 CB TYR	118	56. 473 44. 586 56. 819 44. 903	12. 837 11. 402	1.00 29.52	A	C
ATOM	681 CG TYR 682 CD1 TYR	118 118	56. 819 44. 903 55. 922 45. 572	10. 573	1.00 29.31	A	Č
ATOM ATOM	682 CD1 TYR 683 CE1 TYR	118	56. 236 45. 838	9. 239	1.00 28.13	A	č
ATOM	684 CD2 TYR	118	58.040 44.510	10. 864	1.00 28.81	A	č
ATOM	685 CE2 TYR	118	58. 362 44. 769	9. 541	1.00 27.91	A	č
mou	200 JDB 1110						

734 0

ATOM

GLN

123

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(Continued) FIG. 4-15 8.735 1.00 28.04 C 45.431 ATOM 686 CZ TYR 118 57.459 0 7.427 1.00 29.86 **ATOM** 687 OH TYR 118 57.792 45.681 C 1.00 31.53 C 57.641 46.572 13.863 A 688 TYR 118 ATOM 47.763 13.550 1.00 32.24 A 0 689 0 TYR 118 57.683 **ATOM** 14.295 1.00 32.40 N 58.708 45.903 A N ASN 119 690 ATOM 14.459 1.00 33.64 C 60.008 46.557 A CA ASN 119 **ATOM** 691 C 1.00 35.42 60.511 47.128 13.131 Α CB ASN 119 ATOM 692 C 1.00 36.36 ASN 119 61.069 46.066 12.207 Α **ATOM** 693 CG OD1 ASN 119 61.95845.306 12.584 1.00 37.66 A 0 ATOM 694 60.560 46.021 10.983 1.00 37.41 N ND2 ASN A **ATOM** 119 695 \mathbb{C} 59.875 47.697 15.464 1.00 34.07 A **ATOM** ASN 119 696 C 0 15.348 1.00 34.50 A ASN 60.548 48.719 **ATOM** 697 0 119 TYR N 58.996 47.514 16.443 1.00 33.92 A ATOM 698 N 120 17.472 1.00 33.38 C 120 58.741 48.517 Α **ATOM** 699 CA TYR 57.510 48.097 18.290 1.00 33.40 A C **ATOM** CB TYR 120 700 48.870 1.00 33.30 A C ATOM TYR 120 57.290 19.569 701 CG 58.029 \mathbb{C} CD1 TYR 48.582 20.715 1.00 33.37 120 A **ATOM** 702 C 49.284 21.902 1.00 34.88 CE1 TYR 120 57.818 Α **ATOM** 703 C 56.333 49.886 19.636 1.00 33.62 Α ATOM 704 CD2 TYR 120 C 1.00 32.73 CE2 TYR 120 56.114 50.596 20.813 Α **ATOM** 705 CZTYR 120 56.859 50.289 21.944 1.00 35.24 Α C ATOM 706 56.643 0 ATOM 0H TYR 120 50.977 23.121 1.00 37.51 A 707 59.933 48.772 18.396 1.00 33.12 A C C **ATOM** 708 TYR 120 0 47.849 1.00 33.80 TYR 120 60.472 19.007 Α **ATOM** 709 0 60.330 50.038 18.491 1.00 31.69 N **ATOM** 710 N VAL 121 Α C CA VAL 121 61.441 50.446 19.343 1.00 30.32 Α ATOM 711 50.845 18.504 1.00 30.75 A C **ATOM** 712 CB VAL 121 62.672 C 1.00 28.68 CG1 VAL 121 63.853 51.140 19.420 A **ATOM** 713 CG2 VAL 49.736 17.525 1.00 29.00 C 121 63.013 Α **ATOM** 714 C 61.008 51.645 20.190 1.00 29.83 Α **ATOM** 715 С VAL 121 19.670 0 **ATOM** 716 0 VAL 121 60.788 52.738 1.00 30.47 A N 717 N LYS 122 60.889 51.434 21.495 1.00 28.18 **ATOM** A CA LYS 122 60.464 52, 488 22.404 1.00 27.02 C 718 ATOM Α C CB LYS 122 60.214 51.910 23.799 1.00 23.73 A **ATOM** 719 CG 24.819 1.00 21.38 LYS 52.954 A C 720 122 59.793 ATOM CD LYS 122 59.573 52.354 26.191 1.00 20.47 ATOM 721 Α LYS C CE 59.078 53.406 27.174 1.00 19.23 **ATOM** 722 122 Α N LYS 60.062 54.510 27.346 1.00 18.20 A **ATOM** 723 NZ 122 22.528 C 1.00 27.64 A **ATOM** 724 C LYS 122 61.46053.635 0 **ATOM** 725 0 LYS 122 62.658 53.464 22.315 1.00 28.10 A 22.860 1.00 27.23 N 60.947 54.813 N GLN Α **ATOM** 726 123 C 55.979 23.071 1.00 27.82 727 CA GLN 123 61.791 A **ATOM** 1.00 28.29 C CB GLN 61.607 57.034 21.974 Α **ATOM** 728 123 62.537 58. 227 22.164 1.00 28.94 729 CG GLN 123 Α **ATOM** 59.308 21.131 C 1.00 29.91 **ATOM** 730 CD GLN 123 62.339 Α 0 123 61.218 59.744 20.889 1.00 32.37 A OE1 GLN **ATOM** 731 N 1.00 30.94 **ATOM** 732 NE2 GLN 123 63.431 59.761 20.524 Α C 123 61.385 56, 545 24.428 1.00 26.89 Α 733 C GLN ATOM

SUBSTITUTE SHEET (RULE 26)

61.837

56.036

25.453

1.00 27.03

0

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(Continued)

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Τ.	1	U.	4	T O

ATOM	735	N	TRP	124	60.522	57. 564	24.444	1.00 23.89	· A	N
ATOM	736		TRP	124	60.081	58.149	25.713	1.00 24.21	Α	C
							25. 572	1.00 23.25	Ä	Ċ
ATOM	737		TRP	124	59.886	59.665				
ATOM	738	CG	TRP	124	61.052	60.357	24. 934	1.00 19.79	A	C
ATOM	739	CD2	TRP	124	62.444	60.061	25.127	1.00 19.03	Α	C
ATOM	740		TRP	124	63.175	60.913	24.270	1.00 19.13	Α	C
					63. 143	59. 157	25.936	1.00 15.51	Ä	Č
ATOM	741	-	TRP	124						Č
ATOM	742	CD1	TRP	124	60.999	61.350	24.006	1.00 18.84	A	
ATOM	743	NE1	TRP	124	62.270	61.690	23.597	1.00 18.74	Α	N
ATOM	744	CZ2	TRP	124	64. 571	60.885	24.196	1.00 17.77	Α	C
ATOM	745		TRP	124	64. 533	59.129	25.860	1.00 15.41	Α	С
		CH2	TRP	124	65. 229	59. 986	24.996	1.00 17.07	Ā	C
ATOM	746							1.00 24.57		č
ATOM	747	C	TRP	124	58. 787	57. 494	26. 209		A	
ATOM	748	0	TRP	124	58.490	56. 350	25.861	1.00 25.71	A	0
ATOM	749	N	ARG	125	58.013	58. 218	27.013	1.00 24.36	A	N
ATOM	750	CA	ARG	125	56.779	57.670	27.567	1.00 23.36	Α	C
ATOM	751	CB	ARG	125	56. 189	58.621	28.609	1.00 23.81	Α	C
	752	CG	ARG	125	54. 953	58.065	29. 308	1.00 23.85	A	Č
ATOM										č
ATOM	753	CD	ARG	125	54. 273	59. 129	30. 143	1.00 26.24	A	
ATOM	754	NE	ARG	125	55.090	59.579	31. 269	1.00 25.99	Ą	N
ATOM	755	CZ	ARG	125	55. 293	58.867	32.372	1.00 26.04	A	C
ATOM	756	NH1	ARG	125	56.051	59.357	33. 347	1.00 24.42	Α	N
ATOM	757		ARG	125	54. 735	57.668	32.500	1.00 25.19	Α	N
				125	55. 706	57. 324	26. 541	1.00 24.00	Ä	· Ĉ
ATOM	758	C	ARG							
ATOM	759	0	ARG	125	54. 935	56. 387	26. 752	1.00 25.04	A	0
ATOM	760	N	HIS	126	55. 651	58.063	25.436	1.00 23.33	Α	N
ATOM	761	CA	HIS	126	54. 649	57.800	24.403	1.00 22.86	A	C
ATOM	762	CB	HIS	126	53.649	58.943	24.353	1.00 21.14	A	C
ATOM	763	CG	HIS	126	52.987	59. 224	25.662	1.00 22.35	A	C
						60. 316	26. 463	1.00 21.51	A	č
ATOM	764		HIS	126	53.027					
ATOM	765		HIS	126	52. 137	58. 329	26. 274	1.00 22.03	A	N
ATOM	766	CE1	HIS	126	51.679	58.859	27.395	1.00 23.59	A	C
ATOM	767	NE2	HIS	126	52.202	60.064	27.532	1.00 22.48	A	N
ATOM	768	C	HIS	126	55.222	57. 599	22.995	1.00 24.43	A	C
ATOM	769	Ŏ	HIS	126	54. 599	56.947	22.153	1.00 23.99	A	0
ATOM	770	N	SER	127	56.401	58. 163	22.744	1.00 23.89	A	Ň
									_	C
ATOM	771	CA	SER	127	57.039	58. 072	21.434	1.00 24.38	A	^
ATOM	772	CB	SER	127	58.050	59. 213	21. 267	1.00 23.49	A	Ü
ATOM	773	0G	SER	127	58.909	59.311	22.387	1.00 23.05	Α	0
ATOM	774	C	SER	127	57. 737	56.748	21.146	1.00 24.40	Α	C
ATOM	775	Ō	SER	127	58.167	56.050	22.061	1.00 26.55	Α	0
	776	N	TYR	128	57. 841	56.420	19.861	1.00 22.67	Ä	Ň
ATOM									A	C
ATOM	777	CA	TYR	128	58. 501	55. 207	19.403	1.00 22.06		0
ATOM	778	CB	TYR	128	57.787	53. 962	19. 928	1.00 21.99	A	C
ATOM	779	CG	TYR	128	56.413	53.712	19. 331	1.00 22.49	A	C
ATOM	780	CD1	TYR	128	55. 257	54.112	20.003	1.00 23.20	Α	C
ATOM	781	CE1	TYR	128	53.992	53.857	19.487	1.00 19.81	Α	C
	782		TYR	128	56. 267	53.049	18. 109	1.00 20.70	Ä	Č
ATOM									A	Č
ATOM	783	CEZ	TYR	128	55.007	52. 791	17. 580	1.00 20.87	n	U

		F	IG. 4-	1 7			(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	784 CZ TYR 785 OH TYR 786 C TYR 787 O TYR 788 N THR 789 CA THR 790 CB THR 791 OG1 THR 792 CG2 THR 793 C THR 794 O THR 795 N ALA 796 CA ALA 797 CB ALA 796 CA ALA 797 CB ALA 797 CB ALA 798 C ALA 799 O ALA 800 N SER 801 CA SER 801 CA SER 802 CB SER 803 OG SER 804 C SER 805 O SER 806 N TYR 807 CA TYR 808 CB TYR 809 CG TYR 809 CG TYR	128 53. 83 128 52. 63 128 58. 50 128 57. 80 129 59. 32 129 59. 36 129 60. 72 129 61. 73 129 59. 00 129 59. 16 130 58. 63 130 58. 13 130 58. 13 130 58. 13 131 57. 93 131 57. 73 131 57. 73 131 56. 29 131 56. 29 131 56. 29 132 54. 34 132 53. 53 132 53. 64	72 53. 197 14 52. 946 19 55. 160 10 55. 922 28 54. 281 10 54. 125 23 54. 474 10 55. 951 10 52. 675 10 52. 675 10 51. 062 10 50. 983 17 51. 988 17 51. 988 18 49. 767 19 49. 540 19 49. 540 10 48. 779 11 49. 061 12 50. 357 14 49. 061 15 50. 357 16 50. 357 17 49. 351 18 49. 061 19 50. 357 19 51. 046	18. 279 17. 776 17. 882 17. 224 17. 320 15. 874 15. 245 15. 844 15. 419 15. 580 16. 457 14. 337 13. 943 14. 618 12. 445 11. 740 11. 965 10. 556 10. 059 10. 022 10. 426 11. 397 9. 232 9. 029 9. 156 10. 507	1. 00 22. 39 1. 00 19. 88 1. 00 22. 84 1. 00 24. 63 1. 00 25. 24 1. 00 27. 54 1. 00 33. 01 1. 00 28. 79 1. 00 24. 85 1. 00 22. 29 1. 00 24. 54 1. 00 25. 98 1. 00 25. 98 1. 00 27. 15 1. 00 27. 15 1. 00 27. 62 1. 00 27. 15 1. 00 27. 62 1. 00 27. 17 1. 00 27. 17 1. 00 27. 00 1. 00 27. 16 1. 00 28. 28 1. 00 27. 16 1. 00 28. 28 1. 00 27. 16 1. 00 28. 28 1. 00 27. 16 1. 00 28. 28 1. 00 27. 16	A A A A A A A A A A A A A A A A A A A	Continued) C C C C C C C C C C C C C C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	810 CD1 TYR 811 CE1 TYR 812 CD2 TYR 813 CE2 TYR 814 CZ TYR 815 OH TYR 816 C TYR 817 O TYR 818 N ASP 819 CA ASP 820 CB ASP 821 CG ASP 821 CG ASP 822 OD1 ASP 823 OD2 ASP 824 C ASP 825 O ASP 826 N ILE 827 CA ILE 828 CB ILE 829 CG2 ILE 830 CG1 ILE 831 CD1 ILE 831 CD1 ILE	132 52. 69 132 54. 7 132 54. 8 132 53. 8 132 53. 8 132 54. 7 133 53. 0 133 52. 6 133 54. 7 133 54. 5 133 54. 7 133 54. 7 133 55. 4 134 50. 5 134 49. 1 134 49. 1 134 49. 4 134 49. 2 134 49. 2 134 49. 2 134 49. 2 134 49. 2 134 49. 2 134 49. 2 134 49. 2 134 49. 6	90 51. 483 14 51. 908 22 52. 549 56 52. 333 40 52. 976 71 48. 418 94 48. 639 28 47. 604 29 46. 956 47 45. 519 41 45. 436 73 46. 042 00 44. 756 25 46. 952 67 46. 384 79 47. 598 44 47. 652 32 48. 816 21 48. 954 21 50. 095 32 51. 277	11. 500 12. 735 10. 785 12. 016 12. 985 14. 198 7. 680 6. 712 7. 631 6. 392 6. 314 5. 721 4. 649 6. 321 6. 321 6. 321 6. 321 6. 321 6. 322 5. 315 5. 157 4. 269 4. 752 3. 846 4. 524	1. 00 24. 00 1. 00 23. 00 1. 00 22. 89 1. 00 21. 43 1. 00 22. 58 1. 00 21. 69 1. 00 28. 72 1. 00 29. 54 1. 00 29. 99 1. 00 31. 05 1. 00 31. 90 1. 00 33. 52 1. 00 35. 83 1. 00 30. 39 1. 00 33. 36 1. 00 28. 05 1. 00 25. 68 1. 00 23. 81 1. 00 22. 12 1. 00 23. 64 1. 00 27. 46	A A A A A A A A A A A A A A A A A A A	C C C C C C C C C C C C C C C C C C C

ATOM

881

CB

ARG

140

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(Continued) FIG. 4-18 0 3.521 1.00 27.19 Α 45.894 134 49.171 **ATOM** 833 0 ILE 1.00 29.43 N 45.805 5.127 TYR 135 47.599 Α ATOM 834 N C 44.588 4.628 1.00 30.54 Α TYR 135 46.985 **ATOM** 835 CA 1.00 33.25 C A 135 46.800 43.588 5.772 ATOM 836 CB TYR ${\bf C}$ TYR 46.276 42.242 5.343 1.00 35.66 A CG 135 **ATOM** 837 4.731 1.00 37.89 A 41.311 47.113 CD1 TYR 135 ATOM 838 Č A 40.068 4.319 1.00 40.13 46.634 **ATOM** 839 CE1 TYR 135 $_{\rm C}^{\rm C}$ A 41.903 1.00 37.34 840 CD2 TYR 135 44.939 5.535 **ATOM** 40.666 5.126 1.00 40.17 A CE2 TYR 135 44.444 **ATOM** 841 C 45.296 39.751 4.518 1.00 41.67 A 135 CZ TYR **ATOM** 842 0 1.00 42.54 A 4.105 44.811 38.526 0H TYR 135 **ATOM** 843 C Α 45.629 44.990 4.057 1.00 30.05 TYR 135 ATOM 844 C 0 44.870 45.705 4.704 1.00 28.31 A **ATOM** 845 0 TYR 135 N 1.00 31.33 A N **ASP** 136 45.341 44.536 2.841 **ATOM** 846 1.00 33.02 C 44.083 44.837 2.168 A 847 CA ASP 136 **ATOM** C 44.323 44,857 0.655 1.00 32.51 A **ASP** 136 848 CB **ATOM** 1.00 33.01 C 45.095 -0.146A 43.057 CG ASP 136 ATOM 849 0 45.872 1.00 31.21 Α 43.115 -1.121ATOM 850 OD1 ASP 136 0 1.00 34.97 Α **ATOM** 851 OD2 ASP 136 42.009 44.500 0.181 C C **ASP** 136 43.019 43.797 2.549 1.00 35.55 A 852 **ATOM** 42.822 42.810 1.846 1.00 36.12 A 0 **ASP** 136 **ATOM** 853 0 1.00 38.03 N 42.341 44.040 3.669 A N LEU 137 854 **ATOM** C 41.303 43.150 4.192 1.00 40.58 Α LEU 137 **ATOM** 855 CA C CB 40.445 43.892 5.225 1.00 40.10 LEU 137 Α **ATOM** 856 1.00 39.13 C 6.477 **ATOM** 857 CG LEU 137 41.160 44.413 Α C 137 40.206 45.257 7.307 1.00 37.54 Α CD1 LEU **ATOM** 858 43.243 7.286 1.00 38.91 Α C CD2 LEU 137 41.686 **ATOM** 859 40. 392 42.536 1.00 42.88 C 137 3.134 A 860 LEU **ATOM** C 1.00 43.41 0 40.038 41.362 3.225 137 Α ATOM 861 0 LEU 1.00 45.42 N 39.997 43.322 2.141 Α 862 N ASN 138 ATOM 1.00 48.50 C ATOM 863 CA ASN 138 39.132 42.796 1.093 Α CB ASN 138 38.537 43.936 0.264 1.00 49.71 A C **ATOM** 864 37.127 44.291 0.697 1.00 50.83 A C ASN 138 **ATOM** CG 865 44.555 1.871 1.00 51.97 A 0 36.873 **ATOM** OD1 ASN 138 866 1.00 52.74 N 138 36.202 44.296 -0. 254 Α **ATOM** 867 ND2 ASN 39.884 41.824 0.191 1.00 49.47 C C ASN 138 Α ATOM 868 39.642 40.619 0.240 1.00 50.62 Α 0 **ATOM** 869 0 ASN 138 42.346 -0.6261.00 50.26 A N 139 40.794 **ATOM** 870 N LYS 41.581 41.507 -1.5261.00 51.09 A C CA LYS 139 **ATOM** 871 42.374 -2.3821.00 51.15 C 42.510 A **ATOM** 872 CB LYS 139 C -3.2121.00 53.38 A CG LYS 139 41.785 43.427 **ATOM** 873 C 42.753 44.331 -3.9741.00 54.25 A **ATOM** 874 CD LYS 139 C -5.0211.00 56.31 A ATOM 875 CE LYS 139 43.550 43.564 44.447 1.00 56.39 N 44.453 -5.817NZ LYS 139 **ATOM** 876 1.00 51.63 C 42.413 40.528 -0.703A C **ATOM** 877 LYS 139 0 1.00 51.80 -1.251**ATOM** 878 0 LYS 139 43.148 39, 708 1.00 51.49 N 42.288 40.624 0.618 Α 879 N ARG 140 **ATOM** 1.00 51.71 39.768 1.534 Α C 43.025 880 CA **ARG** 140 **ATOM**

SUBSTITUTE SHEET (RULE 26)

38.408

1.642

42.338

1.00 53.88

C

										(Continued)
					FΙ	G. 4	- 19			(Continued)
ATOM	882	CG	ARG	140	40. 911	38. 495	2. 157	1.00 57.36	A	C
ATOM	883	CD	ARG	140	40. 257	37. 128	2. 211	1.00 60.02	A	C
ATOM	884	NE	ARG	140	40. 936	36. 235	3. 142	1.00 62.76	A	N
ATOM	885	CZ	ARG	140	40.633	34. 950	3. 294	1.00 64.87	A	C
ATOM	886 887	NH1 NH2		140 140	39.661 41.298	34. 409 34. 206	2. 570 4. 169	1.00 66.83 1.00 65.62	A A	N N
ATOM ATOM	888	C	ARG	140	44. 464	39. 603	1.066	1.00 50.02	A	C
ATOM	889	0	ARG	140	44. 992	38. 496	1.000	1.00 50.23	A	0
ATOM	890	N	GLN	141	45. 096	40. 723	0.741	1.00 49.82	A	Ň
ATOM	891	CA	GLN	141	46. 473	40. 707	0. 268	1.00 48.70	A	Ċ
ATOM	892	CB	GLN	141	46. 487	40. 815	-1.260	1.00 50.32	Ä	Č,
ATOM	893	CG	GLN	141	47. 774	40. 348	-1.909	1.00 55.02	A	Ċ '
ATOM	894	CD	GLN	141	47.640	40.179	-3.413	1.00 57.33	A	С
ATOM	895	0E1		141	48.582	39.756	-4.088	1.00 57.97	Α	0
ATOM	896	NE2	GLN	141	46.465	40.509	-3.947	1.00 58.85	Α	N
ATOM	897	C	GLN	141	47. 293	41.837	0.898	1.00 46.02	Α	С
ATOM	898	0	GLN	141	46. 761	42.880	1.274	1.00 45.33	A	0
ATOM	899	N	LEU	142	48. 594	41.610	1.013	1.00 43.34	Α	N
ATOM	900	CA	LEU	142	49. 505	42. 578	1.605	1.00 41.50	A	C
ATOM	901	CB	LEU	142	50. 638	41.824	2. 296	1.00 41.17	A	C
ATOM	902	CG	LEU	142	51.489	42. 501	3. 359	1.00 42.33	A	C
ATOM	903	CD1		142	52.443	41.463	3.922	1.00 42.24	A	C
ATOM	904 905	CD2 C	LEU	142	52. 254	43.677	2.772	1.00 42.66	A	C
ATOM ATOM	906	0	LEU	142 142	50.062 50.557	43. 498 43. 030	0.520 -0.506	1.00 40.87 1.00 41.57	A A	C 0
ATOM	907	N	ILE	143	49. 978	44. 806	0. 748	1.00 41.37	A	N N
ATOM	908	CA	ILE	143	50.466	45. 789	-0.217	1.00 37.17	A	Č
ATOM	909	CB	ILE	143	49. 921	47. 202	0. 104	1.00 36.58	A	č
ATOM	910	CG2		143	50. 486	48. 225	-0.874	1.00 35.56	Ä	č
ATOM	911	CG1		143	48. 398	47. 197	0.030	1.00 34.64	A	č
ATOM	912	CD1		143	47.777	48. 494	0.468	1.00 37.28	Ā	Č
ATOM	913	C	ILE	143	51.985	45.843	-0.209	1.00 36.06	A	C
ATOM	914	0	ILE	143	52.603	45.859	0.849	1.00 36.63	Α	0
ATOM	915	N	THR	144	52. 592	45.882	-1.386	1.00 35.40	Α	N
ATOM	916	CA	THR	144	54.046	45. 933	-1.459	1.00 35.79	Α	С
ATOM	917	CB	THR	144	54.616	44.654	-2.124	1.00 35.59	A	С
ATOM	918	0G1	THR	144	54. 192	44. 592	-3. 491	1.00 37.13	A	0
ATOM	919	CG2		144	54. 121	43. 415	-1.403	1.00 33.21	A	C
ATOM	920	C	THR	144	54. 515	47. 152	-2. 243	1.00 35.43	A	C
ATOM	921	0	THR	144	55. 700	47. 311	-2.511	1.00 36.45	A	0
ATOM	922	N	GLU	145	53. 577	48.015	-2.602	1.00 36.27	A	N
ATOM ATOM	923 924	CA CB	GLU GLU	145 145	53. 891 52. 962	49. 214 49. 297	-3.369 -4.586	1.00 36.32 1.00 38.36	A A	C
ATOM	925	CG	GLU	145 145	53. 553	49. 297	-4. 560 -5. 875	1.00 38.30	A	C C
ATOM	926	CD	GLU	145	54.667	49. 639	-6.418	1.00 42.00	A	Ċ
ATOM	927	0E1		145	55. 745	49. 705	-5.779	1.00 45.49	A	Ö
ATOM	928	0E2		145	54. 456	50. 283	-7.476	1.00 45.56	A	ŏ
ATOM	929	C	GLU	145	53. 775	50. 496	-2.544	1.00 35.06	Ä	č
ATOM	930	0	GLU	145	52.874	50.635	-1.715	1.00 34.22	A	0

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	FIG. 4-20										
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	931 N GLU 14 932 CA GLU 14 933 CB GLU 14 934 CG GLU 14 935 CD GLU 14 936 OE1 GLU 14 937 OE2 GLU 14 938 C GLU 14 939 O GLU 14 939 O GLU 14 940 N ARG 14 941 CA ARG 14 942 CB ARG 14 942 CB ARG 14 943 CG ARG 14 944 CD ARG 14 945 NE ARG 14 945 NE ARG 14 946 CZ ARG 14 947 NH1 ARG 14 948 NH2 ARG 14 948 NH2 ARG 14 950 O ARG 14 951 N ILE 14 953 CB ILE 14 953 CB ILE 14 953 CB ILE 14 953 CB ILE 14 955 CG1 ILE 14 955 CG1 ILE 14 955 CG1 ILE 14 957 C ILE 14 958 O ILE 14 957 C ILE 14 958 O ILE 14 959 N PRO 16 960 CD PRO 16 961 CA PRO 16 962 CB PRO 16 963 CG PRO 16 964 C PRO 16 965 O PRO 16 966 N ASN 18 967 CA ASN 18 968 CB ASN 18 969 CG ASN 18 969 CG ASN 18 970 OD1 ASN 18 971 ND2 ASN 18 972 C ASN 18	5 54.699 52.706 -2.079 1.00 32.54 53.594 53.608 -2.630 1.00 33.84 53.708 53.924 -4.107 1.00 33.18 54.992 54.651 -4.455 1.00 32.11 55.677 55.129 -3.528 1.00 32.11 55.309 54.754 -5.660 1.00 35.19 54.495 52.521 -0.579 1.00 32.26 53.644 53.172 0.031 1.00 32.38 755.185 51.357 1.437 1.00 32.99 755.992 50.107 1.774 1.00 31.91 755.999 47.649 1.963 1.00 34.66 757.415 47.539 1.650 1.00 37.64 757.844 46.143 3.421 1.00 39.76 758.623 52.483 2.363 1.00 39.79 756.6440 53.330 2.002 1.00 29.74<	(Continued) A								
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	970 OD1 ASN 19 971 ND2 ASN 19 972 C ASN 19 973 O ASN 19 974 N ASN 19 975 CA ASN 1976 CB ASN 1	60 60. 749 49. 215 7. 530 1. 00 36. 40 60 62. 612 49. 319 6. 271 1. 00 36. 52 60 61. 336 53. 245 8. 900 1. 00 30. 50 60 61. 583 54. 348 8. 394 1. 00 31. 20 61 61. 387 53. 022 10. 208 1. 00 28. 46 61 61. 734 54. 078 11. 154 1. 00 28. 87 61 63. 137 54. 622 10. 877 1. 00 30. 74	A N								
ATOM ATOM ATOM	978 OD1 ASN 1	61 64. 213 53. 571 11. 048 1. 00 34. 06 51 64. 360 52. 678 10. 219 1. 00 36. 24 51 64. 965 53. 666 12. 139 1. 00 37. 62	A O A N								

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(Continued)	
(Communication)	

ATOM 980 C ASN 151 60.734 55.230 11.111 1.00 28.16 A C ATOM 981 0 ASN 151 61.118 56.400 11.112 1.00 28.85 A O ATOM 982 N THR 152 59.450 54.895 11.064 1.00 26.20 A N ATOM 983 CA THR 152 59.450 54.895 11.064 1.00 26.27 A N ATOM 983 CA THR 152 57.351 55.125 9.099 1.00 25.27 A C ATOM 985 OGI THR 152 57.351 55.125 9.099 1.00 25.27 A C ATOM 985 OGI THR 152 57.351 55.125 9.099 1.00 25.27 A C ATOM 986 CG2 THR 152 56.004 56.466 10.538 1.00 23.99 A C ATOM 986 CG2 THR 152 57.351 55.125 9.099 1.00 25.27 A C ATOM 987 C THR 152 57.351 55.125 9.099 1.00 25.27 A C ATOM 988 O THR 152 57.393 55.476 13.340 1.00 23.46 A C ATOM 988 N CLN 153 58.134 57.600 12.471 1.00 23.46 A C ATOM 989 N CLN 153 58.134 57.600 12.271 1.00 22.30 A N ATOM 990 CA GLN 153 58.501 59.534 14.063 1.00 25.67 A C ATOM 991 CB GLN 153 58.501 59.534 14.063 1.00 20.67 A C ATOM 992 CG GLN 153 60.092 59.543 13.906 1.00 13.74 A C ATOM 993 CD GLN 153 60.092 59.543 13.906 1.00 13.74 A C ATOM 994 CEI GLN 153 60.092 59.543 13.906 1.00 13.74 A C ATOM 995 CE CLN 153 60.095 60.896 61.260 12.233 1.00 12.70 A O ATOM 997 CE CLN 153 60.495 60.889 61.260 12.233 1.00 12.70 A O ATOM 998 N CLN 153 56.600 58.5112 14.495 1.00 20.90 A N ATOM 999 CA GLN 153 56.605 58.799 15.683 1.00 19.36 A O ATOM 999 CA TRP 154 55.565 58.299 13.531 1.00 20.90 A N ATOM 999 CA TRP 154 55.373 59.897 15.683 1.00 19.36 A O ATOM 999 CA TRP 154 55.373 59.897 15.942 1.00 22.43 A C ATOM 999 CA TRP 154 55.373 59.897 15.942 1.00 22.43 A C ATOM 1002 CD2 TRP 154 55.256 58.299 13.531 1.00 20.90 A N ATOM 1002 CD2 TRP 154 55.256 58.799 15.683 1.00 19.36 A O ATOM 1002 CD2 TRP 154 55.2173 57.902 16.947 1.00 22.93 A C ATOM 1002 CD2 TRP 154 55.2173 57.902 16.947 1.00 22.93 A C ATOM 1002 CD2 TRP 154 55.256 58.797 10.840 1.00 22.97 A C ATOM 1002 CD2 TRP 154 55.256 58.797 10.840 1.00 21.90 A C ATOM 1002 CD2 TRP 154 55.2773 57.902 16.947 1.00 22.97 A C ATOM 1002 CD2 TRP 154 55.2773 57.391 15.697 1.00 22.93 A C ATOM 1002 CD2 TRP 154 55.2773 57.391 15.942 1.00 21.99 A C ATOM 1002 CD2 TRP 154 55.2773 57.343 12.703 1.00 21.90 A						FΙ	G. 4	- 21			(Cor
ATOM 981 O ASN 151 61.118 56.400 11.112 1.00 28.85 A O ATOM 982 N THR 152 59.450 54.895 11.064 1.00 28.27 A N ATOM 983 CA THR 152 59.450 54.895 11.064 1.00 28.27 A N C ATOM 985 GG THR 152 57.119 55.389 10.399 1.00 25.27 A C ATOM 986 CG2 THR 152 56.004 56.466 10.538 1.00 23.99 A C ATOM 986 CG2 THR 152 56.004 56.466 10.538 1.00 23.99 A C ATOM 988 O THR 152 57.351 55.125 9.009 1.00 24.18 A O ATOM 988 O THR 152 56.004 56.466 10.538 1.00 23.99 A C ATOM 988 O THR 152 56.004 56.466 10.538 1.00 23.99 A C ATOM 988 O THR 152 57.933 55.476 13.340 1.00 25.16 A O ATOM 989 N CLN 153 58.134 57.600 12.271 1.00 22.30 A N ATOM 989 N CLN 153 58.134 57.600 12.271 1.00 22.30 A N ATOM 991 CB CLN 153 58.501 59.534 14.063 1.00 20.67 A C ATOM 991 CB CLN 153 60.002 59.543 13.906 1.00 13.74 A C ATOM 992 CG CLN 153 60.092 59.543 13.906 1.00 13.74 A C ATOM 993 CD CLN 153 60.092 59.543 13.906 1.00 13.74 A C ATOM 994 CBI CLN 153 60.095 61.524 14.066 1.00 14.57 A C ATOM 995 NEZ CLN 153 60.495 60.853 13.331 1.00 14.57 A C ATOM 995 NEZ CLN 153 60.495 60.853 13.331 1.00 14.57 A C ATOM 996 C CLN 153 56.460 58.112 14.495 1.00 20.53 A C ATOM 997 O CLN 153 56.460 58.112 14.495 1.00 20.53 A C ATOM 999 CA TRP 154 55.556 58.229 13.531 1.00 20.90 A N ATOM 999 CA TRP 154 55.556 58.229 13.531 1.00 20.90 A N ATOM 999 CA TRP 154 55.556 58.229 13.531 1.00 20.90 A N ATOM 999 CA TRP 154 55.556 58.229 13.531 1.00 20.90 A N ATOM 990 CB TRP 154 55.556 58.229 13.531 1.00 20.90 A N ATOM 990 CB TRP 154 55.556 58.29 13.531 1.00 20.90 A N ATOM 990 CB TRP 154 55.556 58.29 13.531 1.00 20.90 A N ATOM 1000 CB TRP 154 55.556 58.29 13.531 1.00 20.90 A N ATOM 1001 CG TRP 154 51.291 59.5930 14.923 1.00 21.90 A C ATOM 1002 CD2 TRP 154 51.291 59.5930 14.923 1.00 21.90 A C ATOM 1002 CD2 TRP 154 51.291 59.5930 14.923 1.00 21.90 A C ATOM 1004 CB TRP 154 51.291 59.595 11.5976 1.00 22.22 A C ATOM 1006 CB TRP 154 51.291 59.595 11.5976 1.00 22.23 A C ATOM 1007 CZ TRP 154 51.291 59.595 11.5976 1.00 22.20 A C ATOM 1007 CZ TRP 154 51.291 59.595 11.5977 1.00 22.20 A C ATOM 1010 CT TRP 154	ATOM	980	С	ASN	151				1.00 28.16	A	С
ATOM 983 CA THR 152 58.415 55.911 11.041 1.00 24.74 A C ATOM 984 CB THR 152 57.119 55.389 10.399 1.00 25.27 A C ATOM 985 CG1 THR 152 57.351 55.125 9.009 1.00 24.18 A C ATOM 986 CG2 THR 152 56.004 56.426 10.538 1.00 23.99 A C ATOM 987 C THR 152 56.004 56.426 10.538 1.00 23.99 A C ATOM 988 O THR 152 57.933 55.476 13.340 1.00 25.16 A C ATOM 988 O THR 152 57.933 55.476 13.340 1.00 25.16 A C ATOM 988 N GLN 153 58.134 57.620 12.721 1.00 22.30 A N ATOM 990 CA GLN 153 57.916 58.129 14.061 1.00 20.67 A C ATOM 991 CB GLN 153 57.916 58.129 14.061 1.00 19.09 A C ATOM 992 CG GLN 153 60.002 59.543 13.906 1.00 13.74 A C ATOM 993 CD GLN 153 60.089 61.260 12.233 1.00 14.57 A C ATOM 994 OB1 GLN 153 60.089 61.260 12.233 1.00 12.70 A O ATOM 995 NB2 GLN 153 60.089 61.260 12.233 1.00 12.70 A O ATOM 997 C GLN 153 66.460 58.112 14.465 1.00 10.81 A N ATOM 997 C GLN 153 66.460 58.121 14.495 1.00 20.53 A C ATOM 999 CA THR 154 55.556 58.229 13.531 1.00 2.090 A N ATOM 999 CA TRP 154 54.131 58.213 13.831 1.00 19.36 A C ATOM 999 CA TRP 154 55.556 58.229 13.531 1.00 2.090 A N ATOM 999 CA TRP 154 54.131 58.213 13.831 1.00 2.090 A N ATOM 999 CA TRP 154 54.131 58.213 13.831 1.00 2.22 A C ATOM 1002 CD2 TRP 154 53.373 59.498 14.550 1.00 22.43 A C ATOM 1002 CD2 TRP 154 51.695 58.791 15.942 1.00 22.43 A C ATOM 1002 CD2 TRP 154 51.695 58.791 15.942 1.00 22.95 A C ATOM 1003 CB2 TRP 154 51.695 58.791 15.942 1.00 22.95 A C ATOM 1003 CB2 TRP 154 51.695 58.791 15.942 1.00 22.95 A C ATOM 1005 CD1 TRP 154 51.263 57.309 17.847 1.00 22.95 A C ATOM 1006 NEI TRP 154 53.642 58.291 15.976 1.00 22.22 A C ATOM 1007 C22 TRP 154 50.315 59.687 15.942 1.00 22.95 A C ATOM 1008 CD3 TRP 154 51.263 57.309 17.847 1.00 22.95 A C ATOM 1009 CH2 TRP 154 53.642 58.791 15.976 1.00 22.95 A C ATOM 1001 C TRP 154 53.642 58.766 17.784 1.00 22.97 A C ATOM 1010 C TRP 154 53.642 58.767 11.384 1.00 21.43 A C ATOM 1010 C TRP 154 53.642 58.767 11.384 1.00 21.43 A C ATOM 1010 C TRP 154 53.642 58.767 11.384 1.00 21.34 A C ATOM 1010 C TRP 154 53.642 58.767 11.384 1.00 21.34 A C ATOM 1010 C TR						61.118	56.400	11.112	1.00 28.85	Α	
ATOM 985 OG1 THR 152 57.351 55.389 10.399 1.00 25.277 A C ATOM 985 OG1 THR 152 57.351 55.125 9.009 1.00 24.18 A O C ATOM 986 CG2 THR 152 56.004 56.426 10.538 1.00 23.99 A C ATOM 987 C THR 152 58.139 56.319 12.474 1.00 23.46 A C ATOM 988 O THR 152 57.933 55.476 13.340 1.00 25.16 A O C ATOM 989 N GLN 153 58.134 57.620 12.721 1.00 22.30 A N ATOM 990 CA GLN 153 57.916 58.129 14.063 1.00 20.67 A C ATOM 991 CB GLN 153 60.002 59.543 13.906 1.00 13.74 A C ATOM 992 CG GLN 153 60.002 59.543 13.906 1.00 13.74 A C ATOM 993 CD GLN 153 60.002 59.543 13.906 1.00 13.74 A C ATOM 993 CD GLN 153 60.002 59.543 13.906 1.00 13.74 A C ATOM 994 OB1 GLN 153 60.495 60.853 13.331 1.00 14.57 A C ATOM 995 NB2 GLN 153 60.002 59.543 13.906 1.00 13.74 A C ATOM 997 O GLN 153 60.495 60.853 13.331 1.00 14.57 A C ATOM 999 CC GLN 153 60.495 60.853 13.331 1.00 14.57 A C ATOM 999 NB2 GLN 153 60.495 60.853 13.331 1.00 12.70 A O ATOM 999 NB2 GLN 153 56.163 57.979 15.683 1.00 19.36 A O ATOM 999 CC GLN 153 56.460 58.112 14.495 1.00 20.53 A C ATOM 999 CA TRP 154 55.556 58.229 13.531 1.00 20.090 A N ATOM 999 CA TRP 154 55.556 58.229 13.531 1.00 20.90 A N ATOM 999 CA TRP 154 53.733 59.498 14.550 1.00 22.243 A C ATOM 1001 CG TRP 154 53.733 59.498 14.550 1.00 22.22 A C ATOM 1001 CG TRP 154 53.735 59.837 15.942 1.00 23.62 A C ATOM 1004 CB3 TRP 154 53.735 59.837 15.942 1.00 23.62 A C ATOM 1004 CB3 TRP 154 50.135 59.987 15.942 1.00 23.62 A C ATOM 1005 CD1 TRP 154 53.136 60.228 14.308 1.00 24.478 A N ATOM 1007 CZ TRP 154 59.136 57.399 17.847 1.00 22.95 A C ATOM 1006 NEI TRP 154 53.645 58.575 18.257 11.518 1.00 21.90 A C ATOM 1007 CZ TRP 154 53.645 58.556 18.259 13.10 12.00 22.94 A C ATOM 1008 CZ TRP 154 53.645 58.575 11.518 1.00 21.474 A C ATOM 1010 CG TRP 154 53.645 58.575 11.518 1.00 21.34 A C ATOM 1010 CG TRP 154 53.645 58.759 11.5.976 1.00 22.97 A C ATOM 1005 CD1 TRP 154 53.645 58.759 11.5.916 1.00 22.97 A C ATOM 1010 CG TRP 154 53.645 58.759 11.5.916 1.00 22.97 A C ATOM 1010 CG TRP 154 53.645 58.759 11.5.910 10.00 22.97 A C ATOM 1010 CG TRP 154 53.645 58.75	ATOM	982	N	THR		59.450				Α	
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ATOM 1027 CA TRP 157 44.423 56.985 9.627 1.00 21.45 A C								9. 577			
ATUM 1028 CB TRP 157 43.426 55.825 9.765 1.00 21.88 A C											Č
	ATOM	1028	CB	TKP	157	43. 426	55. 825	9. 765	1.00 21.88	A	C

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(Continued) FIG. 4-22 ATOM 1029 CG TRP 157 43.995 54.450 9.599 1.00 20.88 C 53.800 **ATOM** 1030 CD2 TRP 157 44.315 8.364 1.00 18.96 C 52. 531 CE2 TRP 44.843 1.00 19.67 1031 157 8.686 ATOM A C 44.208 **ATOM** 1032 CE3 TRP 157 54.168 7.019 1.00 17.93 Α C 157 44.328 **ATOM** 1033 CD1 TRP 53. 571 10.592 1.00 20.82 C Α 44.838 ATOM 1034 NE1 TRP 157 52.417 10.052 1.00 21.01 Α N 1035 CZ2 TRP 45.265 **ATOM** 157 51.626 7.708 1.00 19.12 C A 1036 **ATOM** CZ3 TRP 157 44.627 53.267 6.046 1.00 19.76 C A CH2 TRP **ATOM** 1037 157 45.149 52.011 6.397 1.00 19.30 C A 9.801 **ATOM** 1038 C TRP 157 43.650 58.276 1.00 23.03 A C ATOM 1039 0 TRP 157 43.750 58.917 10.843 1.00 25.03 A 0 ATOM 1040 42.889 N SER 158 58.663 8.784 1.00 23.17 N A **ATOM** 1041 158 42.064 59.855 8.889 CA SER 1.00 23.44 C Α 1042 ATOM CB 41.667 1.00 22.82 SER 158 60.362 7.502 C A **ATOM** 1043 0G SER 158 41.208 59.311 6.679 1.00 23.84 Α 0 1044 C **ATOM SER** 158 40.845 59.377 9.678 1.00 23.86 C Α **ATOM** 1045 0 SER 158 40.613 58.176 9.781 1.00 24.35 0 Α **ATOM** 1046 N **PRO** 159 40.056 60.301 10.247 1.00 24.17 Α N **ATOM** 1047 CD PR₀ 159 40.136 61.762 10.114 1.00 24.24 C A 1048 ATOM CA PR₀ 159 38.876 59.922 11.029 1.00 23.40 Α C **ATOM** 1049 **PRO** 159 38. 270 61.264 CB 11.419 1.00 23.45 C Α 62. 214 CG PRO **ATOM** 1050 159 39.427 11.353 1.00 24.19 C Α **ATOM** 1051 C **PRO** 159 37.901 59.090 10.224 C 1.00 25.36 Α **ATOM** 1052 0 **PRO** 58.248 159 37. 191 10.771 1.00 27.14 0 Α **ATOM** 1053 VAL 160 37.878 59.334 N 8.919 1.00 25.28 Α N **ATOM** 1054 CA VAL 36.977 160 58.640 8.014 1.00 23.99 A C ATOM 1055 CB VAL Ċ 160 35. 784 59.545 7.689 1.00 24.54 A **ATOM** 1056 CG1 VAL 160 35.066 59.064 6.449 1.00 26.50 C A 59.559 **ATOM** 1057 CG2 VAL 160 34.834 8.875 1.00 26.15 C Α 37.679 **ATOM** 1058 VAL C 160 58.218 6.730 1.00 23.78 C A **ATOM** 1059 38.570 0 VAL 160 58.908 6.245 1.00 24.51 Α 0 ATOM 1060 N **GLY** 161 37. 268 57.080 6.181 1.00 24.05 A N ATOM 1061 CA **GLY** 37.876 4.962 1.00 22.93 161 56.579 C A 55. 786 1062 ATOM C GLY 161 39.121 5.286 1.00 23.87 C A ATOM 1063 0 **GLY** 161 39.144 55.045 6.269 1.00 24.24 0 Α ATOM 1064 N HIS 55.950 162 40.164 4.476 1.00 25.01 N Α 41.423 **ATOM** 1065 CA HIS 55. 239 162 1.00 25.86 C 4.695 A **ATOM** 1066 CB HIS 41.419 53.923 162 3.920 1.00 26.04 A ${\bf C}$ CG HIS **ATOM** 1067 162 41.075 54.087 2.475 1.00 27.52 A CD2 HIS **ATOM** 1068 162 41.614 54.875 C 1.515 1.00 27.58 A **ATOM** 1069 ND1 HIS 162 40.039 53.402 1.874 1.00 27.77 N A **ATOM** 1070 CE1 HIS 162 39.956 53.764 0.606 1.00 28.51 C A **ATOM** 1071 NE2 HIS 162 40.900 54.656 0.363 1.00 28.82 N A ATOM 1072 C HIS 162 42.660 56.053 4.305 1.00 25.44 C A HIS 43.636 **ATOM** 1073 0 162 55.501 3.794 1.00 24.38 0 A **ATOM** 1074 N LYS 163 42.609 57.364 4.527 1.00 24.47 N Α CA 1075 LYS 163 **ATOM** 43.751 58. 221 4.224 1.00 23.45 C Α ATOM 1076 CB LYS 163 43.372 59.701 4.273 1.00 21.75 C Α CG 1077 LYS 42.528 **ATOM** 163 60.216 C 3.130 1.00 21.55

					T? T	C 1	9 9			(Continued)
					r 1	G. 4	- 23			
ATOM	1078	CD	LYS	163	42. 281	61.706	3. 335	1.00 20.23	Α	C
ATOM	1079	CE	LYS	163	41.464		2. 228	1.00 18.07	Α	C
ATOM	1080	NZ	LYS	163	41.315		2. 422	1.00 20.95	A	N
ATOM	1081	C	LYS	163	44. 781	57. 961	5. 309	1.00 23.44	A	Ċ
ATOM	1082	Ŏ	LYS	163	44. 425		6. 433	1.00 23.42	A	Õ
ATOM	1083	Ň	LEU	164	46.053		4. 979	1.00 23.11	A	N
ATOM	1084	CA	LEU	164	47. 117		5. 950	1.00 23.65	Ā	Ċ
ATOM	1085	CB	LEU	164	48.014		5. 524	1.00 24.35	A	Č
ATOM	1086	ĊĠ	LEU	164	47. 551	55. 351	5.848	1.00 25.57	Ā	Č
ATOM	1087		LEU	164	48. 519		5. 219	1.00 25.59	A	Č
ATOM	1088		LEU	164	47. 497		7. 359	1.00 25.62	Ā	Č
ATOM	1089	C	LEU	164	47.970		6.120	1.00 23.21	A	Ċ
ATOM	1090	0	LEU	164	48. 175		5.177	1.00 24.34	Α	0
ATOM	1091	N	ALA	165	48.456		7. 335	1.00 21.88	A	N
ATOM	1092	CA	ALA	165	49.319		7.649	1.00 21.58	Α	C
ATOM	1093	CB	ALA	165	48.548		8.376	1.00 21.77	Α	C
ATOM	1094	C	ALA	165	50.406		8.545	1.00 22.07	Α	C
ATOM	1095	0	ALA	165	50.115		9.537	1.00 22.91	Α	0
ATOM	1096	N	TYR	166	51.661	60. 208	8. 201	1.00 22.02	A	N
ATOM	1097	CA	TYR	166	52.745	59.697	9.024	1.00 21.73	Α	С
ATOM	1098	CB	TYR	166	53.185		8.520	1.00 22.38	Α	С
ATOM	1099	CG	TYR	166	53.814		7.141	1.00 22.11	Α	C
ATOM	1100	CD1	TYR	166	55.148	58.661	6.964	1.00 21.28	Α	C
ATOM	1101	CE 1	TYR	166	55.733	58.638	5.704	1.00 22.05	Α	C
ATOM	1102	CD2	TYR	166	53.074	57. 949	6.015	1.00 20.67	Α	C
ATOM	1103	CE2	TYR	166	53.648	57. 923	4.753	1.00 20.02	Α	С
ATOM	1104	CZ	TYR	166	54. 981	58. 2 6 8	4.603	1.00 21.75	Α	С
ATOM	1105	OH	TYR	166	55. 566		3. 352	1.00 20.77	Α	0
ATOM	1106	C	TYR	166	53. 927		9.057	1.00 21.64	A	С
ATOM	1107	0	TYR	166	54. 108		8. 157	1.00 21.61	· A	0
ATOM	1108	N	VAL	167	54. 722		10.111	1.00 20.28	A	N
ATOM	1109	CA	VAL	167	55.886		10. 264	1.00 19.16	Α	С
ATOM	1110	CB	VAL	167	55. 924		11.644	1.00 19.56	A	С
ATOM	1111		VAL	167	57. 103		11.731	1.00 18.58	A	С
ATOM	1112		VAL	167	54.609	62. 713	11.916	1.00 18.36	A	C
ATOM	1113	C	VAL	167	57.135		10.078	1.00 20.06	A	C
ATOM	1114	0	VAL	167	57. 287		10.679	1.00 21.80	A	0
ATOM	1115	N	TRP	168	58. 030		9. 233	1.00 19.65	A	N
ATOM	1116	CA	TRP	168	59. 268		8. 964	1.00 19.61	A	C
ATOM	1117	CB	TRP	168	59. 164		7.646	1.00 20.07	A	C
ATOM	1118	CG	TRP	168	60. 387	58. 772	7. 353	1.00 23.12	A	C
ATOM	1119		TRP	168	61.319	59. 011	6. 300	1.00 21.38	Ą	C
ATOM	1120		TRP	168	62. 353		6. 436	1.00 21.58	A	C.
ATOM	1121		TRP	168	61.382	59. 936	5. 256	1.00 21.74	A	C
ATOM	1122		TRP	168	60.873	57. 712	8.066	1.00 22.86	A	Ç
ATOM	1123		TRP	168	62.056	57. 281	7. 521	1.00 21.54	A	N
ATOM	1124		TRP	168	63. 445	58. 012	5. 563	1.00 23.71	- A	C
ATOM	1125		TRP	168	62.468		4. 386	1.00 23.21	A	C
ATOM	1126	CHZ	TRP	168	63. 484	58. 934	4. 546	1.00 22.74	A	С

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(c									(Continued)
					FIG.	4 - 24			(Oommada)
	1100		TID D	1.60	00 400 01	207 0 004	2 1 00 17) 17 A	C
ATOM	1127	C	TRP	168		327 8.906			C
ATOM	1128	0	TRP	168		319 8.187			0 N
ATOM	1129	N	ASN	169		072 9.682			N C
ATOM	1130	CA	ASN	169		969 9.732			C
ATOM	1131	CB	ASN	169		902 8.417			C
ATOM	1132	CG	ASN	169		565 8. 217			C
ATOM	1133		ASN	169		196 7.09			0 N
ATOM	1134		ASN	169		832 9.30			
ATOM	1135	Ç	ASN	169		394 10.00			
ATOM	1136	0	ASN	169		344 9.378			
ATOM	1137	N	ASN	170		522 10.938			
ATOM	1138	CA	ASN	170		817 11.354			
ATOM	1139	CB	ASN	170		679 11.88			
ATOM	1140	CG	ASN	170		193 13. 239			
ATOM	1141		ASN	170		025 13.404			
ATOM	1142		ASN	170		092 14. 210			
ATOM	1143	C	ASN	170		621 10.34			
ATOM	1144	0	ASN	170		815 10.54			
ATOM	1145	N	ASP	171		974 9. 264			
ATOM	1146	CA	ASP	171		643 8. 254			
ATOM	1147	CB	ASP	171		696 6.893			
ATOM	1148	CG	ASP	171		750 6.830			
ATOM	1149		ASP	171		876 7.30			
ATOM	1150		ASP	171		454 6. 29			
ATOM	1151	C	ASP	171		888 8.099			
ATOM	1152	0	ASP	171		690 8. 383			
ATOM	1153	N	ILE	172		585 7.633			
ATOM	1154	CA	ILE	172		983 7.46			
ATOM	1155	CB	ILE	172		966 7.89			
ATOM	1156		ILE	172		329 7. 73			
ATOM	1157		ILE	172		394 9. 350			
ATOM	1158		ILE	172		538 9. 795 530 6.04			
ATOM	1159	C	ILE	172		539 6.04			
ATOM	1160		ILE	172		246 5.08			0
ATOM	1161	N	TYR	173		358 5.92			
ATOM	1162	CA	TYR	173		808 4.62			
ATOM	1163	CB	TYR	173		612 4. 25			
ATOM	1164	CG	TYR	173		921 4.12			
ATOM	1165	CD1		173		978 5. 23			
ATOM	1166	CE1		173		271 5. 100			
ATOM	1167		TYR	173		165 2.87			C
ATOM	1168		TYR	173		460 2.72			C
ATOM	1169	CZ	TYR	173		512 3.83			
ATOM	1170	OH	TYR	173		837 3.67			
ATOM	1171	C	TYR	173		341 4.67			
ATOM	1172	0	TYR	173		008 5.74			
ATOM	1173	N	VAL	174		306 3.51			
ATOM	1174	CA	VAL	174		865 3.44			
ATOM	1175	CB	VAL	174	49. 212 63.	060 3.31	9 1.00 1	8. 88 A	C

(Continued)

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		004	****		10 000	00 504	0 007	1 00 10	07 4	_
ATOM	1176	CG1		174	47. 775	62. 564	3. 207	1.00 19.		C
ATOM	1177	CG2	VAL	174	49.359	63.969	4.534	1.00 20.		C
ATOM	1178	C	VAL	174	49.948	60.928	2.268	1.00 21.	57 A	. C
ATOM	1179	0	VAL	174	50. 485	61.129	1.185	1.00 22.	86 A	0
ATOM	1180		LYS	175	49. 154	59. 891	2.500	1.00 23.		N
	1181		LYS	175	48. 824	58. 934	1.461	1.00 23.		Ċ
ATOM							1.831	1.00 23.		Č
ATOM	1182		LYS	175	49. 275	57. 516				C
ATOM	1183		LYS	175	50. 759	57. 352	2.113	1.00 28.		
ATOM	1184	CD	LYS	175	51.100	55. 895	2.422	1.00 29.		C
ATOM	1185	CE	LYS	175	51.107	55.043	1.163	1.00 29.		C
ATOM	1186	NZ	LYS	175	52.263	55.409	0.291	1.00 31.		N
ATOM	1187	. C	LYS	175	47.314	58.935	1.338	1.00 24.	49 A	C
ATOM	1188	0	LYS	175	46.615	58.606	2.293	1.00 25.	05 A	0
ATOM	1189	N	ILE	176	46.820	59.319	0.166	1.00 24.	77 A	N
ATOM	1190	CA	ILE	176	45. 394	59. 327	-0.102	1.00 24.		С
ATOM	1191	CB	ILE	176	45. 095	60.028	-1.437	1.00 22.		Ċ
		CG2	ILE	176	43. 605	60.073	-1.679	1.00 22.		č
ATOM	1192						-1.423	1.00 21.		Č
ATOM	1193	CG1	ILE	176	45.677	61.443				
ATOM	1194	CD1	ILE	176	45.016	62. 379	-0.424	1.00 23.		C
ATOM	1195	C	ILE	176	44. 995	57.860	-0.211	1.00 26.		C
ATOM	1196	0	ILE	176	43.979	57. 428	0.328	1.00 26.		0
ATOM	1197	N	GLU	177	45.829	57.097	-0.906	1.00 29.		N
ATOM	1198	CA	GLU	177	45.597	55.672	-1.104	1.00 31.	88 A	C
ATOM	1199	CB	GLU	177	45.412	55.380	-2.594	1.00 35.	29 A	C
ATOM	1200	CG	GLU	177	44. 308	56.190	-3.248	1.00 38.	36 A	С
ATOM	1201	CD	GLU	177	42.925	55.776	-2.784	1.00 41.	13 A	C
ATOM	1202	0E1	GLU	177	41.951	56.495	-3.105	1.00 45.		0
ATOM	1203	0E2		177	42.810	54. 730	-2.107	1.00 40.		0
ATOM	1204	C	GLU	177	46. 796	54. 895	-0.569	1.00 31.		Č
ATOM	1205	Õ	GLU	177	47. 940	55. 223	-0.872	1.00 31.		ŏ
ATOM	1206	N	PRO	178	46.544	53. 840	0. 221	1.00 31.		N
						53. 240	0. 438	1.00 31.		C
ATOM	1207	CD	PRO	178	45. 218					Č
ATOM	1208	CA	PRO	178	47. 591	53.000	0.814			
ATOM	1209	CB	PRO	178	46. 796	51.902	1.509	1.00 30.		C
ATOM	1210	CG	PRO	178	45. 567	51.805	0.684	1.00 31.		C
ATOM	1211	C	PRO	178	48. 633	52. 436	-0.150	1.00 29.		C
ATOM	1212	0	PR0	178	49.727	52.062	0. 269	1.00 31.		0
ATOM	1213	N	ASN	179	48. 308	52.379	-1.436	1.00 28.		N
ATOM	1214	CA	ASN	179	49. 251	51.838	-2.409	1.00 27.		С
ATOM	1215	CB	ASN	179	48. 568	50.805	-3. 299	1.00 26.		С
ATOM	1216	CG	ASN	179	47. 474	51.409	-4.144	1.00 25.	74 A	С
ATOM	1217	0D1	ASN	179	46. 494	51.948	-3.626	1.00 26.		0
ATOM	1218		ASN -	179	47. 635	51.329	-5.452	1.00 26.		N
ATOM	1219	C	ASN	179	49. 854	52. 916	-3. 285	1.00 27.		C
ATOM	1220	ŏ	ASN	179	50. 818	52. 670	-4.004	1.00 28.		ŏ
	1221	N	LEU	180	49. 289	54. 115	-3.231	1.00 26.		N
ATOM						55. 200	-4. 050			Č
ATOM	1222	CA	LEU	180	49.805			1.00 20.		C
ATOM	1223	CB	LEU	180	48. 658	56. 125	-4. 456			
ATOM	1224	CG	LEU	180	47. 574	55. 370	-5. 238	1.00 25.	87 A	U

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(Continued)

FIG. 4-26

ATOM	1225	CD1	LEU	180	46.604	56.359	-5.856	1.00 23.58	Α	C
ATOM	1226		LEU	180	48. 224	54.503	-6.328	1.00 22.86	Α	C
						55.996	-3. 391	1.00 25.78	Ä	Č
ATOM	1227	Ç	LEU	180	50. 938					
ATOM	1228	0	LEU	180	51. 185	55.883	-2.185	1.00 23.62	A	0
ATOM	1229	N	PRO	181	51.669	56. 789	-4.194	1.00 24.96	Α	N
ATOM	1230	CD	PRO	181	51.687	56.842	-5.667	1.00 23.41	Α	C
ATOM	1231	CA	PRO	181	52.766	57.580	-3.634	1.00 23.35	A	С
ATOM	1232	CB	PRO	181	53. 403	58. 217	-4.870	1.00 22.16	A	Č
										Č
ATOM	1233	CG	PRO	181	53. 124	57. 201	-5.944	1.00 22.72	A	
ATOM	1234	C	PRO	181	52. 216	58.613	-2.667	1.00 22.15	A	C
ATOM	1235	0	PRO	181	51.144	59. 173	-2.880	1.00 21.88	Α	0
ATOM	1236	N	SER	182	52.954	58.864	-1.601	1.00 21.65	A	N
ATOM	1237	CA	SER	182	52.516	59.829	-0.620	1.00 20.50	A	С
ATOM	1238	CB	SER	182	52. 999	59. 404	0.765	1.00 22.61	Ä	Č
					54. 408		0. 806	1.00 23.55	A	ŏ
ATOM	1239	OG	SER	182		59. 345				
ATOM	1240	C	SER	182	53. 034	61. 222	-0.947	1.00 19.05	A	C
ATOM	1241	0	SER	182	54.003	61.380	-1.687	1.00 17.74	Α	0
ATOM	1242	N	TYR	183	52.366	62.233	-0.402	1.00 17.87	Α	N
ATOM	1243	CA	TYR	183	52. 786	63.606	-0.611	1.00 15.17	Α	C
ATOM	1244	CB	TYR	183	51.595	64.523	-0.832	1.00 12.09	A	C
ATOM	1245	ĊĠ	TYR	183	50.676	64.028	-1.905	1.00 12.54	Ä	Č
ATOM	1246	CD1	TYR	183	49.729	63. 052	-1.625	1.00 8.93	A	č
ATOM	1247	CE1	TYR	183	48. 916	62. 554	-2.610	1.00 11.95	A	C
ATOM	1248	CD2	TYR	183		64. 494	-3. 214	1.00 9.42	A	C
ATOM	1249	CE2	TYR	183	49.961	63.990	-4.218	1.00 10.27	Α	C
ATOM	1250	CZ	TYR	183	49.032	63.019	-3.903	1.00 10.59	Α	C
ATOM	1251	OH	TYR	183	48.205	62.494	-4.867	1.00 14.71	Α	0
ATOM	1252	C	TYR	183	53.532	64.067	0.617	1.00 15.72	Α	C
ATOM	1253	0	TYR	183	53. 208	63.679	1.740	1.00 17.69	A	0
ATOM	1254	Ň	ARG	184	54. 540	64. 893	0.386	1.00 14.64	Ä	Ň
ATOM	1255	CA		184	55. 342	65. 436	1.452	1.00 14.04		C
			ARG						A	
ATOM	1256	CB	ARG	184	56.786	65. 593	0.970	1.00 16.84	A	C
ATOM	1257	CG	ARG	184	57.725	66. 203	1.989	1.00 20.48	A	C
ATOM	1258	CD	ARG	184	59. 170	65.912	1.629	1.00 20.61	Α	C
ATOM	1259	NE	ARG	184	60.095	66.485	2.598	1.00 20.21	A	N
ATOM	1260	CZ	ARG	184	61.407	66.288	2.583	1.00 19.46	Α	C
ATOM	1261	NH1	ARG	184	61.954	65.529	1.650	1.00 17.13	A	N
ATOM	1262		ARG	184	62.170	66.853	3.506	1.00 20.35	Ä	N
ATOM	1263	C	ARG	184	54. 736	66. 779	1.820	1.00 14.10	A	Ċ
ATOM	1264	0	ARG	184	54. 569	67. 650	0.972	1.00 14.71	A	0
ATOM	1265	N	ILE	185	54. 390	66. 937	3.089	1.00 15.27	A	Ŋ
ATOM	1266	CA	ILE	185	53.804	68. 175	3. 572	1.00 14.44	Α	C
ATOM	1267	CB	ILE	185	52.786	67.884	4.692	1.00 16.20	Α	C
ATOM	1268	CG2	ILE	185	52.091	69.175	5.115	1.00 14.78	Α	C
ATOM	1269		ILE	185	51.770	66.842	4. 202	1.00 15.25	Α	C
ATOM	1270		ILE	185	51.021	67. 250	2.947	1.00 12.00	Ä	Č
ATOM	1271	C	ILE	185	54. 847	69. 172	4. 091	1.00 14.33	Ä	Č
ATOM	1272	Ö	ILE	185	54. 647	70. 377	3. 994	1.00 14.33	A	0
ATOM	1273	N	THR	186	55.950	68. 676	4.646	1.00 14.38	A	N

							(Continued)
					FIG. 4-27		(Continued)
ATOM	1274	CA	THR	186			A C
ATOM	1275	CB	THR	186			A C
ATOM	1276	OG1	THR	186			A 0
ATOM	1277		THR	186			A C
ATOM	1278	C	THR	186			A C
ATOM	1279	0	THR	186			A 0
ATOM	1280	N	TRP	187			A N
ATOM	1281	CA	TRP	187			A C
ATOM ATOM	1282 1283	CB CG	TRP TRP	187 187			A C A C
ATOM	1284		TRP	187			A C
ATOM	1285		TRP	187			A C
ATOM	1286		TRP	187			A Č
ATOM	1287		TRP	187			A C ·
ATOM	1288		TRP	187			A N
ATOM	1289		TRP	187			A C
ATOM	1290		TRP	187			A C
ATOM	1291	CH2	TRP	187			A C
ATOM	1292	C	TRP	187	61.607 70.620 5.292 1	.00 15.71	A C
ATOM	1293	0	TRP	187	62. 804 70. 725 5. 053 1		A 0
ATOM	1294	N	THR	188			A N
ATOM	1295	CA	THR	188			A C
ATOM	1296	CB	THR	188			A C
ATOM	1297	0G1		188			A 0
ATOM	1298		THR	188			A C
ATOM	1299	C	THR	188			A C
ATOM	1300	0	THR	188			A 0
ATOM	1301 1302	N	GLY	189			A N
ATOM ATOM	1302	CA C	GLY GLY	189 189			A C
ATOM	1303	0	GLY	189			A C A O
ATOM	1305	N	LYS	190			A N
ATOM	1306	CA	LYS	190			A C
ATOM	1307	CB	LYS	190			A C
ATOM	1308	ĊĠ	LYS	190			A Č
ATOM	1309	CD	LYS	190			A Č
ATOM	1310	CE	LYS	190			A C
ATOM	1311	NZ	LYS	190			A N
ATOM	1312	C	LYS	190			A C
ATOM	1313	0	LYS	190		. 00 18. 41	A 0
ATOM	1314	N	GLU	191			A N
ATOM	1315	CA	GLU	191			A C
ATOM	1316	CB	GLU	191			A C
ATOM	1317	CG	GLU	191			A C
ATOM	1318	CD	GLU	191			A C
ATOM	1319	0E1		191			A 0
ATOM	1320		GLU	191			A 0
ATOM	1321	C	GLU	191			A C
ATOM	1322	0	GLU	191	67. 930 67. 397 15. 156 1.	. 00 22. 21	A 0

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				FIG	÷. 4	- 28				
ATOM	1323 N	ASP	192	66. 262	66. 451	16.320	1.00 21.17	Α	N	
ATOM	1324 CA	ASP	192		67. 246	17.525	1.00 22.27	Α	C	
ATOM	1325 CB	ASP	192		66.880	18.182	1.00 23.92	A	C	
ATOM	1326 CG	ASP	192		65.400	18.510	1.00 25.20	Α	С	
ATOM		ASP	192		64. 775	18.850	1.00 25.70	Α	0	
ATOM		2 ASP	192		64.866	18.438	1.00 26.25	Α	0	
ATOM	1329 C	ASP	192		68.759	17.341	1.00 21.93	A	C	
ATOM	1330 0	ASP	192		69.489	18.145	1.00 22.78	Α	0	
ATOM	1331 N	ILE	193	65. 748	69. 242	16.304	1.00 21.66	A	N	
ATOM	1332 CA	ILE	193	65 ⁻ . 685	70.684	16.071	1.00 20.08	A	C	
ATOM	1333 CB	ILE	193		71.113	15.039	1.00 20.73	Α	С	
ATOM	1334 CG	2 ILE	193		72.567	14.677	1.00 18.91	Α	Č	
ATOM	1335 CG	I ILE	193		70. 889	15.624	1.00 22.58	A	C	
ATOM	1336 CD		193		71. 198	14.671	1.00 26.43	A	Č	
ATOM	1337 C	ILE	193		71.172	15.615	1.00 19.15	A	Ç	
ATOM	1338 0	ILE	193		72.068	16. 220	1.00 19.55	Ą	0	
ATOM	1339 N	ILE	194		70. 594	14. 534	1.00 19.04	Ą	N	
ATOM	1340 CA	ILE	194		70. 967	14.021	1.00 17.41	A	C	
ATOM	1341 CB	ILE	194		71.547	12.587	1.00 18.89	Ą	C	
ATOM		2 ILE	194		71.944	12.095	1.00 16.97	A	C	
ATOM		1 ILE	194		72.750	12.553	1.00 19.26	A	C	
ATOM		1 ILE	194		73.936	13. 395	1.00 16.78	A	C	
ATOM	1345 C	ILE	194		69.702	13.969	1.00 18.22	A	C	
ATOM	1346 0	ILE	194		68.713	13. 349	1.00 17.31	A	0 N	
ATOM	1347 N	TYR	195		69. 726	14.642	1.00 17.31	A	N	
ATOM	1348 CA		195		68. 593	14.639	1.00 16.19	A	C	
ATOM	1349 CB	TYR	195		68.071	16.053	1.00 17.03 1.00 17.58	A A	C	
ATOM	1350 CG		195		67. 776 68. 802	16.893 17.286	1.00 17.38	A	C	
ATOM	1351 CD 1352 CE		195 195		68. 558	18. 145	1.00 16.25	A	Č	
ATOM ATOM		1 11K 2 TYR	195		66. 490	17. 377	1.00 15.45	A	č	
ATOM		2 TYR	195		66. 237	18. 240	1.00 15.14	A	č	
ATOM	1354 CE		195		67. 275	18. 624	1.00 17.41	A	Č	
AŢOM	1356 OH		195		67.041	19.515	1.00 21.26	A	ŏ	
ATOM	1357 C	TYR		••••	69.016	14.047	1.00 16.29	A	Č	
ATOM	1358 0	TYR			69.902	14. 586	1.00 15.85	Ä	ŏ	
ATOM	1359 N	ASN			68.380	12.942	1.00 15.27	Ā	N	
ATOM	1360 CA				68.656	12. 286	1.00 12.88	· A		
ATOM	1361 CB				68.894	10.790	1.00 13.47	A	C C C	
ATOM	1362 CG				70.133	10.489	1.00 14.66	Α	C	
ATOM		1 ASN			71.261	10.678	1.00 10.34	Α	0	ť
ATOM		2 ASN			69.927	10.013	1.00 15.26	Α	N	
ATOM	1365 C	ASN			67.438	12.457	1.00 14.12	Α	C	
ATOM	1366 0	ASN			66.347	12.044	1.00 16.31	A	0	
ATOM	1367 N	GLY			67.613	13.065	1.00 14.48	Α	N	
ATOM	1368 CA			53.622	66.488	13. 231	1.00 15.17	Α	C	7
ATOM	1369 C	GLY	197		65.638	14. 458	1.00 15.48	A	C	•
ATOM	1370 0	GLY			64.799	14.815	1.00 15.55	A	0	
ATOM	1371 N	ILE	198	55.023	65.846	15.098	1.00 16.49	A	N	

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							4.0.00	1 00 10 50		
ATOM	1372	CA	ILE	198	55.378	65.097	16. 298	1.00 16.59	Α	C
ATOM	1373	CB	ILE	198	56.425	63. 991	16.011	1.00 18.21	Α	C
ATOM	1374		ILE	198	55.874	63.013	14.987	1.00 18.51	Α	C
			ILE			64.602	15.494	1.00 17.86	Ä	Č
ATOM	1375			198	57.724					
ATOM	1376		ILE	198	58. 798	63.565	15. 214	1.00 19.35	A	C
ATOM	1377	C	ILE	198	55.946	66.057	17.318	1.00 15.95	Α	C
ATOM	1378	0	ILE	198	56.507	67.091	16.966	1.00 17.63	Α	0
ATOM	1379	Ň	THR	199	55. 809	65.700	18.583	1.00 15.42	Α	N
			THR	199	56. 264	66.547	19.672	1.00 16.68	Ä	Ċ
ATOM	1380	CA								č
ATOM	1381	CB	THR	199	55. 374	66.316	20.908	1.00 17.40	A	
ATOM	1382	0G1	THR	199	55.462	64.944	21.301	1.00 18.82	Α	0
ATOM	1383	CG2	THR	199	53.924	66.619	20.583	1.00 15.72	Α	C
ATOM	1384	C	THR	199	57.716	66.334	20.076	1.00 16.00	Α	C
ATOM	1385	Ŏ	THR	199	58. 317	65.325	19.734	1.00 16.12	Α	0
ATOM	1386	N	ASP	200	58. 276	67. 301	20. 801	1.00 16.87	Ä	Ň
ATOM	1387	CA	ASP	200	59.649	67. 193	21. 289	1.00 15.49	A	C
ATOM	1388	CB	ASP	200	60.315	68.576	21.418	1.00 14.82	Α	C
ATOM	1389	CG	ASP	200	59. 681	69.446	22.491	1.00 17.16	A	C
ATOM	1390	0D1	ASP	200	58. 517	69.190	22.873	1.00 16.41	Α	0
ATOM	1391	0D2		200	60. 348	70.403	22.945	1.00 15.97	Α	0
ATOM	1392	C	ASP	200	59,496	66.515	22.641	1.00 15.54	Ä	Č
ATOM	1393	0	ASP	200	58. 388	66.118	22.999	1.00 17.01	A	0
ATOM	1394	N	TRP	201	60. 581	66. 381	23. 395	1.00 15.10	A	N
ATOM	1395	CA	TRP	201	60.504	65.699	24.672	1.00 13.14	A	C
ATOM	1396	CB	TRP	201	61.885	65.619	25.326	1.00 14.90	Α	C
ATOM	1397	CG	TRP	201	61.905	64.679	26.510	1.00 15.25	Α	C
ATOM	1398	CD2	TRP	201	61.412	64. 953	27. 828	1.00 13.65	Ä	č
										č
ATOM	1399	CE2	TRP	201	61.500	63. 753	28. 564	1.00 13.52	A	
ATOM	1400	CE3		201	60. 902	66.096	28. 456	1.00 11.78	A	C
ATOM	1401	CD1	TRP	201	62.269	63.360	26.507	1.00 13.81	A	C
ATOM	1402	NE1	TRP	201	62.025	62.799	27.733	1.00 13.64	A	N
ATOM	1403	CZ2	TRP	201	61.096	63.661	29.897	1.00 14.03	Α	C
ATOM	1404	CZ3	TRP	201	60. 502	66.009	29. 778	1.00 12.04	Ä	Č
	1405	CH2	TRP	201	60.601	64. 797	30. 486	1.00 14.87	Ä	č
ATOM										
ATOM	1406	C	TRP	201	59. 529	66. 327	25.662	1.00 14.42	A	C
ATOM	1407	0	TRP	201	58. 635	65.656	26. 175	1.00 13.63	A	0
ATOM	1408	N	VAL	202	59. 691	67.615	25.931	1.00 15.14	A	N
ATOM	1409	CA	VAL	202	58.830	68.265	26.911	1.00 14.23	Α	C
ATOM	1410	CB	VAL	202	59.402	69.639	27. 330	1.00 12.99	Α	C
ATOM	1411		VAL	202	59.010	70. 716	26. 322	1.00 11.02	Ä	Č
									A	č
ATOM	1412		VAL	202	58. 947	69. 963	28. 753			
ATOM	1413	C	VAL	202	57. 365	68. 401	26.518	1.00 15.76	A	C
ATOM	1414	0	VAL	202	56.497	68. 404	27. 391	1.00 18.74	A	0
ATOM	1415	N	TYR	203	57. 072	68.518	25. 226	1.00 15.58	A	N
ATOM	1416	CA	TYR	203	55. 676	68.606	24.805	1.00 14.25	Α	C
ATOM	1417	CB	TYR	203	55. 556	69.078	23. 354	1.00 14.63	A	Ċ
	1418	CG		203	55. 227	70. 542	23. 227	1.00 12.35	Ä	č
ATOM			TYR							Č
ATOM	1419	CD1		203	56. 231	71.508	23. 193	1.00 11.91	A	
ATOM	1420	CE1	TYR	203	55. 920	72.867	23. 108	1.00 11.20	Α	С

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(Continued) FIG. 4-30 C 70.966 23.177 1.00 12.17 A **ATOM** 1421 CD2 TYR 203 53.902 C 72.314 23.099 1.00 10.57 Α 1422 CE2 TYR 203 53.579 ATOM 9.67 C 73.259 23.061 1.00 A 1423 CZTYR 203 54.588 ATOM 54.259 74.586 22.970 1.00 7, 05 0 TYR Α 1424 OH 203 ATOM C 24.951 1.00 14.92 Α 55.024 67.234 TYR 203 **ATOM** 1425 C 0 25.406 1.00 15.28 Α. 53.896 67.124 **ATOM** 1426 0 TYR 203 N 24.570 1.00 16.35 Α ATOM 1427 N GLU 204 55.744 66.185 **GLU** 204 55.222 64.826 24.684 1.00 16.96 A C 1428 CA **ATOM** 24.130 C 56.238 63.812 1.00 14.28 Α 204 1429 CB **GLU** ATOM C 55.928 62.380 24.540 1.00 14.97 Α GLU 204 **ATOM** 1430 ÇG C 1.00 19.54 23.947 Α 56.872 61.345 ATOM 1431 CD GLU 204 24.271 0 56.697 60.144 1.00 18.49 A **ATOM** 1432 OE1 GLU 204 1.00 18.73 0 OE2 GLU 204 57.778 61.714 23.160 Α 1433 **ATOM** 54.868 64.431 26.128 1.00 18.02 Α C 204 **ATOM** 1434 C **GLU** 26.388 1.00 17.48 0 GLU 53.816 63.848 Α 1435 0 204 **ATOM** 55.757 64.761 27.059 1.00 18.67 N GLU Α N 205 **ATOM** 1436 28.459 1.00 20.30 C 55.589 64.409 A **ATOM** 1437 CA GLU 205 C 64.250 29.096 1.00 20.92 A **ATOM** 1438 CB GLU 205 56.970 1.00 24.62 C 1439 CG GLU 205 56.958 64.03530.592 Α **ATOM** 56.563 62.625 30.974 1.00 28.17 A C CD GLU 1440 205 **ATOM** 0 56.398 62.355 32.182 1.00 32.15 OE1 GLU 205 A 1441 **ATOM** 0 61.778 30.069 1.00 31.11 A OE2 GLU 205 56, 424 **ATOM** 1442 C 54.760 65.362 29.319 1.00 22.25 **ATOM** 1443 C GLU 205 Α 64.915 30.164 1.00 22.34 0 **ATOM** 1444 0 GLU 205 53.996 Α **GLU** 206 54.902 66.66629.107 1.00 22.70 Α N 1445 N **ATOM** 67.632 29.939 1.00 23.19 Α C 54.202 **ATOM** 1446 CA GLU 206 C 55.203 68.667 30.453 1.00 25.39 A CB GLU 206 **ATOM** 1447 C 68.088 31.080 1.00 27.87 Α 56.466 **ATOM** 1448 CG GLU 206 C 32.345 CD GLU 206 56.188 67.307 1.00 29.45 A **ATOM** 1449 1.00 29.92 0 57.160 66.855 32.987 Α **ATOM** 1450 OE1 GLU 206 OE2 GLU 206 55.000 67.144 32.696 1.00 29.12 Α 0 1451 **ATOM** 68.378 29.324 1.00 24.91 C 53.024 Α C **GLU** 206 **ATOM** 1452 0 30.051 1.00 24.03 206 52.175 68.885 A **GLU ATOM** 1453 0 27.999 N 52.957 68.452 1.00 25.41 Α ATOM 1454 N VAL 207 C 51.880 69.199 27.375 1455 VAL 207 1.00 25.29 Α ATOM CA 1.00 25.95 C 52.444 70.235 26.398 Α **ATOM** 1456 CB VAL 207 CG1 VAL 207 51.324 71.114 25.876 1.00 28.49 A 1457 **ATOM** C 71.080 27.092 1.00 26.77 Α 207 53.496 **ATOM** 1458 CG2 VAL C 207 50.801 68.409 26.653 1.00 26.09 1459 A **ATOM** C VAL 0 1.00 27.62 68.703 26.813 VAL 207 49.617 Α **ATOM** 1460 0 N 51.194 67.412 25.865 1.00 26.41 A PHE 208 **ATOM** 1461 N C 1.00 26.03 **ATOM** 1462 PHE 208 50.228 66.620 25. 105 Α CA C 50.557 66.676 23.607 1.00 27.43 A 1463 CB PHE 208 **ATOM** C 22.962 1,00 28.64 50.234 67.994 A CG 208 **ATOM** 1464 PHE C 1.00 29.07 22.679 68.911 A **ATOM** 1465 CD1 PHE 208 51.234 Č 1.00 30.01 CD2 PHE 208 48.918 68.328 22.660 Α **ATOM** 1466 C 70.142 22.104 1.00 30.28 50.929 A ATOM 1467 CE1 PHE 208 C 48.604 22.086 1.00 30.23 Α 69.556 1468 CE2 PHE 208 ATOM C 1.00 30.40

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70.464

49.612

ATOM

1469

CZ PHE

208

21.809

ATOM

1518

CD2 TRP

215

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(Continued) FIG. 4-31 **ATOM** PHE 25.506 C 1470 C 208 50.082 65.163 1.00 26.13 1471 PHE 208 64.471 **ATOM** 0 49.215 24.985 1.00 27.79 0 A 1472 209 N **ATOM** N SER 50.918 64.687 26.421 1.00 26.62 A 1473 SER 209 50.852 63.293 26.848 1.00 25.74 C **ATOM** CA Α C 49.645 63.059 27.743 **ATOM** 1474 CB SER 209 1.00 24.80 A 1475 0G SER 209 49.871 63.629 29.014 1.00 29.47 Α 0 ATOM C ATOM 1476 C SER 209 50.773 62.377 25.642 1.00 25.50 A ATOM 1477 0 SER 209 50.278 61.249 25.716 1.00 25.72 0 A N ATOM 1478 N ALA 210 51.272 62.875 24.524 1.00 23.72 A 1479 CA 210 51.263 62.112 23.299 1.00 22.80 $_{\rm C}^{\rm C}$ **ATOM** ALA Α **ATOM** 1480 CB ALA 210 49.977 62.364 22.530 1.00 20.62 A **ATOM** 1481 210 52.455 62.560 22.492 1.00 21.87 C C ALA Α 22.703 0 **ATOM** 1482 0 ALA 210 52.986 63.644 1.00 22.09 A 211 52.863 21.558 N **ATOM** 1483 N TYR 61.719 1.00 21.57 A **ATOM** 1484 CA 211 54.000 62.009 20.718 CCCCCCCTYR 1.00 21.42 Α 54.725 **ATOM** 1485 CB TYR 211 60.711 20.405 1.00 19.58 Α ATOM 1486 CG TYR 211 55.921 60.870 19.528 1.00 16.81 Α 1487 CD1 TYR 211 61.870 19.770 ATOM 56.853 1.00 16.07 Α **ATOM** 1488 CE1 TYR 211 58.002 61.971 19.001 1.00 18.18 A CD2 TYR **ATOM** 1489 211 56.160 59.976 18.489 1.00 17.91 A **ATOM** 1490 CE2 TYR 211 57.306 60.065 17.716 1.00 18.80 A **ATOM** 1491 CZ TYR 211 58. 221 61.063 17.979 1.00 18.36 Α **ATOM** 1492 0HTYR 211 59.360 61.149 17. 224 1. 00 23. 65 0 Α Ċ **ATOM** 1493 C TYR 211 53. 588 62.689 19.428 1.00 22.96 Α 1494 211 ATOM 0 TYR 54.365 63.443 18.837 0 1.00 25.79 A 1495 N 62.433 N **ATOM** SER 212 52.365 18.983 1.00 20.96 A 1496 **ATOM** CASER 212 51.918 63.033 17.746 C 1.00 19.56 A **ATOM** 1497 CB SER 212 50.835 17.090 Ċ 62.175 1.00 20.97 Α **ATOM** 1498 0G SER 212 49.635 62.208 17.829 1.00 21.79 0 Α ATOM 1499 212 C C SER 51.397 64.439 17.959 1.00 18.50 Α **ATOM** 1500 0 SER 212 50.933 64.789 19.040 1.00 16.31 0 Α **ATOM** 1501 N ALA 213 51.493 65.236 16.901 N 1.00 17.84 A **ATOM** 1502 CA ALA 213 51.036 66.610 16.903 1.00 16.02 Α ${\bf C}$ CB **ATOM** 1503 ALA 213 52.193 67.548 17.224 1.00 14.16 Α **ATOM** 1504 C ALA 213 50.429 66.935 15.526 1.00 15.57 C Α 14.833 **ATOM** 1505 0 ALA 213 50.857 67.862 1.00 13.25 0 Α **ATOM** 1506 N LEU 214 49.448 66.132 15.129 1.00 14.75 N Α **ATOM** 1507 CA LEU 214 48.734 66.339 13.874 C 1.00 16.09 A **ATOM** LEU 49.353 1508 CB 214 65.517 12.735 ${\rm C} \\ {\rm C} \\ {\rm C}$ 1.00 16.40 A CG LEU **ATOM** 1509 214 49.482 63.999 12.823 1.00 17.01 A **ATOM** 1510 CD1 LEU 214 48.135 63.342 12.628 1.00 18.97 A 1511 CD2 LEU 50.434 C ATOM 214 63.535 11.742 1.00 16.98 A 47.273 C **ATOM** 1512 C LEU 214 65.963 14.124 1.00 16.65 A 46.966 **ATOM** 1513 0 LEU 214 64.933 14.728 1.00 18.12 0 A **ATOM** 1514 TRP 46.366 N 215 66.811 13.666 1.00 16.16 A N **ATOM** 1515 CA TRP 215 44.959 66.590 13.907 1.00 14.69 C Α 1516 TRP 44.471 67.663 Č CB 215 ATOM 14.863 1.00 15.49 Α 1517 CG TRP 215 45. 230 ATOM 67.669 16.145 1.00 17.52 C A

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16.403

1.00 17.74

A

46.482

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				F	[G. 4	- 3 2			(Continued)
ATOM	1519	CE2		15 46. 852		17. 729	1.00 17.50	A	C
ATOM ATOM	1520 1521	CE3		15 47. 329 15 44. 904		15. 643 17. 289	1.00 18.21 1.00 15.79	A	C C
ATOM	1522			15 45.873		18. 243	1.00 13.73	A A	N N
ATOM	1523	CZ2		15 48.033		18. 318	1.00 18.06	A	C
ATOM	1524	CZ3		48.50		16. 228	1.00 18.96	A	
ATOM	1525			15 48. 844		17.555	1.00 18.21	Ä	C C C
ATOM	1526			15 44.110		12.661	1.00 15.55	Ā	Ċ
ATOM	1527			15 43. 869	9 67.668	12.090	1.00 16.18	Α	0
ATOM	1528			l 6 43.646	65.430	12.244	1.00 15.31	Α	N
ATOM	1529			6 42.793		11.069	1.00 16.40	Α	C
ATOM	1530			16 42.494		10. 739	1.00 16.43	A	C
ATOM	1531		IRP 21			10.002	1.00 17.38	A	C
ATOM	1532	CD2				8. 599	1.00 17.01	A	C
ATOM ATOM	1533 1534	CE2 T				8. 320	1.00 17.25	A	C
ATOM	1535	CD1 7				7. 549 10. 508	1.00 17.09	A	C C C C C C
ATOM	1536	NEI I				9. 501	1.00 18.55 1.00 18.07	A A	N N
ATOM	1537	CZ2 1				7. 036	1.00 15.07	A	
ATOM	1538	CZ3 1			63.729	6. 270	1.00 17.06	A	C C C
ATOM	1539		TRP 21	6 44. 794	62.734	6.027	1.00 17.07	Ä	Č
ATOM	1540		TRP 21			11.355	1.00 17.17	Ä	č
ATOM	1541	0 7	TRP 21			12.487	1.00 18.00	Ä	0
ATOM	1542		SER 21	7 40.847		10.334	1.00 18.39	Α	N
ATOM	1543		SER 21	39. 552		10.523	1.00 19.62	Α	C
ATOM	1544		SER 21	7 39. 257	68. 225	9.392	1.00 20.31	Α	C
ATOM	1545		SER 21	7 39. 234	67.589	8. 133	1.00 24.00	A	0
ATOM	1546		SER 21			10.550	1.00 20.47	A	C,
ATOM ATOM	1547 1548		SER 21 PRO 21		64.994	10.110	1.00 20.32	A	0
ATOM	1549		PRO 21		66.369 67.650	11. 074 11. 598	1.00 20.82 1.00 20.28	A	N C
ATOM	1550		PRO 21		65.339	11. 154	1.00 20.28	A A	C C
ATOM	1551		RO 21	8 35.033	66.148		1.00 21.68	A	Č
ATOM	1552		PRO 21			12. 353	1.00 21.12	A	Č
ATOM	1553		PRO 21			9. 950	1.00 23.46	Ä	č
ATOM	1554	0 P	PRO 21			10.107	1.00 25.13	Ā	Ö
ATOM	1555			9 35.909	64.948	8.756	1.00 22.93	Α	N
ATOM	1556		ASN 21			7.600	1.00 22.31	Α	C
ATOM	1557		ISN 21			6. 631	1.00 22.48	Α	C
ATOM	1558		ISN 21			5.903	1.00 24.12	A	C
ATOM	1559	OD1 A				5. 760	1.00 26.01	A	0
ATOM ATOM	1560	ND2 A				5. 411	1.00 26.27		N
ATOM	1561 1562		ASN 21 ASN 21			6.871	1.00 21.20	A	C
ATOM	1563		LY 22			5. 760 7. 499	1.00 20.94 1.00 18.33	A A	0 N
ATOM	1564		LY 22			6. 941	1.00 18.33	A	N C
ATOM	1565		LY 22			5. 853	1.00 11.31	A	C
ATOM	1566		LY 22			5. 375	1.00 20.28	Ä	Ŏ
ATOM	1567		HR 22			5. 447	1.00 17.57	Ä	Ň

										(Con	tinued)
					FΙ	G. 4	- 33				
40014	1500	0.4	mr.m	001	00 051	00.015	4 400	1 00 15 00		0	
ATOM	1568	CA	THR	221	39.654	66. 917	4. 408	1.00 15.80	Ą	C	
ATOM	1569	CB	THR	221	38. 540	67.942	4. 112	1.00 15.67	A	C	
ATOM	1570	0G1		221	37. 410	67. 269	3. 550	1.00 16.41	A	0	
ATOM	1571	CG2		221	39.019	69.004	3. 147	1.00 12.96	A	C	
ATOM	1572	C	THR	221	40.903	67.674	4.833	1.00 16.70	A	C	
ATOM	1573	0	THR	221	41.884	67. 753	4. 088	1.00 16.98	Α	0	
ATOM	1574	N	PHE	222	40.864	68.238	6.033	1.00 15.92	Α	N	
ATOM	1575	CA	PHE	222	41.999	69.001	6.539	1.00 15.88	A	C	
ATOM	1576	CB	PHE	222	41.508	70.253	7.262	1.00 15.20	A	C	
ATOM	1577	CG	PHE	222	40. 939	71.305	6.356	1.00 14.35	A	С	
ATOM	1578		PHE	222	39. 569	71.542	6.323	1.00 11.89	A	C	
ATOM	1579		PHE	222	41.782	72.097	5.571	1.00 14.45	A	C	
ATOM	1580	CE1	PHE	222	39.046	72.550	5.533	1.00 13.50	Α	C	
ATOM	1581	CE2	PHE	222	41.269	73.112	4.771	1.00 12.61	Α	C	
ATOM	1582	CZ	PHE	222	39.897	73.342	4.751	1.00 15.23	Α	C	
ATOM	1583	C	PHE	222	42.907	68.228	7.494	1.00 16.13	Α	C	
ATOM	1584	0	PHE	222	42.467	67.327	8. 211	1.00 16.82	Α	0	
ATOM	1585	N	LEU	223	44. 187	68.582	7.484	1.00 15.93	A	N	
ATOM	1586	CA	LEU	223	45.159	67.983	8.385	1.00 14.81	Α	C	
ATOM	1587	CB	LEU	223	46.199	67.142	7.645	1.00 14.64	Α	C	
ATOM	1588	CG	LEU	223	47.306	66.627	8.584	1.00 14.94	Α	Ċ	
ATOM	1589	CD1	LEU	223	46.696	65.773	9.687	1.00 11.99	A	Ċ	
ATOM	1590		LEU	223	48. 338	65.830	7.808	1.00 11.50	Ā	Č	
ATOM	1591	C	LEU	223	45.848	69.162	9.031	1.00 16.80	Ā	Č	•
ATOM	1592	0	LEU	223	46.398	70.028	8.341	1.00 16.53	Ā	0	
ATOM	1593	· N	ALA	224	45. 790	69.219	10.353	1.00 17.34	Ā	N	
ATOM	1594	CA	ALA	224	46.420	70.308	11.073	1.00 18.47	Ä	Ċ	
ATOM	1595	CB	ALA	224	45.422	70.950	12.029	1.00 17.47	Α	Č	
ATOM	1596	C	ALA	224	47. 596	69.735	11.840	1.00 18.77	A	Ċ	
ATOM	1597	0	ALA	224	47. 587	68.561	12.205	1.00 19.22	Ā	Ō	
ATOM	1598	N	TYR	225	48.614	70.551	12.078	1.00 17.68	Ā	N	
ATOM	1599	CA	TYR	225	49.764	70.068	12.819	1.00 17.56	Ā	C	
ATOM	1600	CB	TYR	225	50.726	69.306	11.891	1.00 16.48	Ā	Č	
ATOM	1601	CG	TYR	225	51.273			1.00 15.05	Ā	Č	
ATOM	1602	CD1	TYR	225	50. 551	70. 235	9. 533	1.00 13.44	A	Č	
ATOM	1603		TYR	225	51.050	70.968	8.456	1.00 9.19	Ā	Č	
ATOM	1604	CD2	TYR	225	52.514	70.740	10.814	1.00 14.42	A	Ċ.	
ATOM	1605	CE2	TYR	225	53.025	71.476	9. 744	1.00 14.09	A	Č	
ATOM	1606	CZ	TYR	225	52. 286	71.583	8.567	1.00 14.11	Ä	Č	
ATOM	1607	OH	TYR	225	52.802	72. 292	7.504	1.00 14.49	Ä	Ŏ	
ATOM	1608	C	TYR	225	50.514	71.182	13.521	1.00 17.79	Ä	Č	
ATOM	1609	0	TYR	225	50. 326	72.359	13. 229	1.00 19.91	Ä	Ö	
ATOM	1610	N	ALA	226	51.358	70.796	14. 462	1.00 17.65	A	Ň	•.
ATOM	1611	CA	ALA	226	52. 164	71.748	15. 201	1.00 17.74	Ä	Ċ	
ATOM	1612	CB	ALA	226	52.060	71.472	16.687	1.00 18.89	Ä	Č	
ATOM	1613	C	ALA	226	53.601	71.575	14. 740	1.00 17.39	Ä	č	
ATOM	1614	0	ALA	226	53.966	70.527	14. 204	1.00 16.05	Ä	Ŏ	
ATOM	1615	N	GLN	227	54.412	72.606	14. 941	1.00 17.45	A	N	
ATOM	1616	CA	GLN	227	55.816	72. 552	14. 555	1.00 16.64	Ä	Ĉ	
						_	1 2. 000	1.00 10.01	•-	-	

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(Continued) FIG. 4-34 C 227 56.096 73.423 13. 331 1.00 15.62 ATOM 1617 CB GLN 73.246 1.00 16.35 C ATOM 1618 CG GLN 227 57.514 12.799 A GLN 227 57.847 74.191 11.666 1.00 14.31 ATOM 1619 CD A **ATOM** 1620 OE1 GLN 227 57.877 75.408 11.851 1.00 18.11 A ATOM 1621 227 58.101 73.639 10.486 1.00 12.45 NE2 GLN N 15.723 56.615 73.073 1.00 16.27 **ATOM** C GLN 227 C 1622 A 56.346 74.159 16.225 1.00 16.33 1623 0 **GLN** 227 0 **ATOM** 72.301 **ATOM** 1624 N PHE 228 57.601 16.158 1.00 17.36 A N 1625 228 58.414 72.717 17.287 1.00 16.81 ATOM CA PHE C 228 58.327 71.686 18.412 1.00 14.62 C **ATOM** 1626 CB PHE A 56.919 71.295 CG PHE 18.758 1.00 14.48 C 1627 228 A ATOM 1628 CD1 PHE 228 56.317 70.196 18.141 1.00 14.37 **ATOM** A 1629 C 56.183 72.036 19.674 CD2 PHE 228 1.00 12.73 **ATOM** A **ATOM** 1630 CE1 PHE 228 55.007 69.840 18.430 1.00 13.56 A C C ATOM 1631 CE2 PHE 228 54.870 71.691 19.971 1.00 14.73 A 228 54.279 70.588 19.348 C **ATOM** 1632 CZ PHE 1.00 15.31 A 1633 59.848 72.922 C \mathbf{c} 228 16.859 1.00 18.12 **ATOM** PHE Α 60.410 **ATOM** 1634 0 PHE 228 72.121 16.112 1.00 17.47 0 A ATOM 1635 N ASN 229 60.413 74.027 17. 335 1.00 20.00 A N **ATOM** 1636 CA ASN 229 61.779 74.435 17.042 1.00 20.87 C 1637 **ATOM** CB ASN 229 61.767 75.857 16.474 1.00 21.57 C Α 76.257 **ATOM** 1638 CG ASN 229 63.086 15.870 1.00 24.35 C A OD1 ASN 75.774 1639 229 64.141 16.289 1.00 26.00 **ATOM** 0 A 1640 ND2 ASN 229 63.025 77.153 14.887 **ATOM** 1.00 25.62 N 18.362 1.00 21.39 1641 229 62.540 74.421 **ATOM** C ASN A C ATOM 1642 0 ASN 229 62.23275.200 19.269 1.00 21.52 0 1643 N **ASP** 230 63.516 73.530 1.00 20.96 **ATOM** 18.481 N A 1644 ASP 64.300 73.444 **ATOM** 230 19.706 1.00 22.78 CA C 64.275 1.00 22.69 1645 CB ASP 230 72.026 20.268 C ATOM Α 1646 CG ASP 230 62.880 71.551 20.580 1.00 22.37 C ATOM Α OD1 ASP 71.015 **ATOM** 1647 230 62.681 21.689 1.00 21.57 A 0 19.713 **ATOM** 1648 OD2 ASP 230 61.993 71.705 1.00 21.82 0 65.734 1649 C 230 73.825 19.412 1.00 24.50 **ATOM ASP** A 73.252 19.979 1650 0 **ASP** 230 66.663 1.00 24.72 **ATOM** Α 0 1651 N 65.904 **ATOM** THR 231 74.803 18.527 1.00 25.87 Α N 67. 228 18.122 **ATOM** 1652 THR 231 75.245 1.00 26.22 CA C A 17.109 1.00 27.87 **ATOM** 1653 CB THR 231 67.149 76.406 C A **ATOM** 1654 OG1 THR 231 66.540 75.947 15.893 1.00 28.62 0 A CG2 THR **ATOM** 1655 231 68.545 76.947 16.813 1.00 26.63 C A C 1656 231 68.099 75.688 19.280 **ATOM** THR 1.00 26.77 C Α 0 **ATOM** 1657 231 69.254 75.277 19.375 THR 1.00 27.34 A 0 **ATOM** 1658 N GLU 232 67.550 76.519 20.163 1.00 25.50 N A **ATOM** 1659 GLU 232 68.329 77.020 21.285 CA 1.00 24.52 A C 68.154 78.526 21.397 **ATOM** 1660 CB GLU 232 1.00 28.36 C A 1661 CG GLU 232 68.615 79.281 20.171 ATOM 1.00 34.72 C A CD GLU 1662 232 68.483 80.780 20.338 1.00 40.02 **ATOM** Α OE1 GLU 68.767 ATOM 1663 232 81.509 19.363 1.00 44.21 0 A 1664 OE2 GLU 232 68.100 81.232 21.444 **ATOM** 1.00 42.26 A 0 **ATOM** 1665°C GLU 232 68.020 76.377 22.627 1.00 22.97

					(Continued)
				FIG. 4-35	(Continueu)
ATOM	1666	O GLU	232	68. 331 76. 942 23. 679 1. 00 20. 81 A	0
ATOM	1667	N VAL	233	67. 416 75. 194 22. 596 1. 00 20. 32 A	N
ATOM ATOM	1668 1669	CA VAL CB VAL	$\begin{array}{c} 233 \\ 233 \end{array}$	67. 091 74. 499 23. 832 1. 00 17. 88 A 65. 853 73. 618 23. 648 1. 00 17. 88 A	C
ATOM	1670	CG1 VAL	$\frac{233}{233}$	65. 853 73. 618 23. 648 1. 00 17. 88 A 65. 522 72. 925 24. 957 1. 00 14. 00 A	C
ATOM	1671	CG2 VAL	233	64. 678 74. 478 23. 160 1. 00 16. 73 A	C
ATOM	1672	C VAL	233	68. 261 73. 642 24. 304 1. 00 16. 00 A	Ç
ATOM	1673	0 VAL	233	68. 694 72. 728 23. 606 1. 00 15. 94 A	Ö
ATOM	1674	N PRO	234	68. 788 73. 927 25. 504 1. 00 14. 51 A	Ň
ATOM	1675	CD PRO	234	68. 313 74. 907 26. 494 1. 00 13. 03 A	Ċ
ATOM	1676	CA PRO	234	69. 914 73. 162 26. 040 1. 00 13. 93 A	Č
ATOM	1677	CB PRO	234	70. 031 73. 677 27. 473 1. 00 12. 63 A	C
ATOM	1678	CG PRO	234	69.517 75.059 27.377 1.00 11.32 A	C
ATOM	1679	C PRO	234	69. 643 71. 663 25. 987 1. 00 16. 20 A	C
ATOM	1680	O PRO	234	68. 487 71. 220 26. 041 1. 00 15. 73 A	0
ATOM	1681	N LEU	235	70. 716 70. 887 25. 900 1. 00 16. 28 A	N
ATOM	1682	CA LEU	235	70. 602 69. 443 25. 825 1. 00 16. 91 A	C
ATOM	1683	CB LEU	235	71.505 68.912 24.718 1.00 18.54 A	C
ATOM	1684	CG LEU	235	71. 267 69. 349 23. 273 1. 00 21. 93 A	C
ATOM	1685	CD1 LEU	235	72. 434 68. 856 22. 412 1. 00 21. 90 A	C
ATOM	1686	CD2 LEU	235	69. 946 68. 790 22. 768 1. 00 19. 17 A	C
ATOM	1687	C LEU	235	70. 990 68. 743 27. 118 1. 00 17. 26 A	C
ATOM	1688	0 LEU	235	71. 939 69. 157 27. 793 1. 00 18. 36 A	0
ATOM	1689	N ILE	236	70. 244 67. 696 27. 472 1. 00 14. 95 A	N
ATOM ATOM	1690 1691	CA ILE CB ILE	$\begin{array}{c} 236 \\ 236 \end{array}$	70. 586 66. 899 28. 644 1. 00 12. 68 A	C
ATOM	1692	CG2 ILE	$\begin{array}{c} 230 \\ 236 \end{array}$	69. 345 66. 245 29. 335 1. 00 10. 50 A 68. 538 65. 433 28. 329 1. 00 9. 32 A	C
ATOM	1693	CG2 ILE	236	68. 538 65. 433 28. 329 1. 00 9. 32 A 69. 806 65. 298 30. 448 1. 00 8. 74 A	C
ATOM	1694	CD1 ILE	236	70. 789 65. 919 31. 427 1. 00 7. 11 A	C
ATOM	1695	C ILE	236	71. 444 65. 802 28. 010 1. 00 12. 84 A	Č
ATOM	1696	0 ILE	236	71.105 65.276 26.942 1.00 10.11 A	ŏ
ATOM	1697	N GLU	237	72. 558 65. 480 28. 650 1. 00 12. 44 A	N
ATOM	1698	CA GLU	237	73. 463 64. 470 28. 128 1. 00 14. 46 A	Ĉ
ATOM	1699	CB GLU	237	74. 767 65. 128 27. 655 1. 00 13. 45 A	Ċ
ATOM	1700	CG GLU	237	74. 554 66. 079 26. 500 1. 00 18. 02 A	С
ATOM	1701	CD GLU	237	75. 845 66. 500 25. 819 · 1. 00 23. 46 A	C
ATOM	1702	OE1 GLU	237	75. 779 67. 016 24. 683 1. 00 25. 80 A	0
ATOM	1703	OE2 GLU	237	76. 928 66. 324 26. 408 1. 00 26. 23 A	0
ATOM	1704	C GLU	237	73. 744 63. 427 29. 191 1. 00 13. 41 A	C
ATOM	1705	O GLU	237	73. 895 63. 752 30. 363 1. 00 14. 43 A	0
ATOM	1706	N TYR	238	73. 801 62. 169 28. 781 1. 00 12. 83 A	N
ATOM	1707	CA TYR	238	74. 052 61. 093 29. 721 1. 00 14. 06 A	C
ATOM	1708	CB TYR	238	72. 810 60. 840 30. 595 1. 00 12. 42 A	· C
ATOM	1709	CG TYR	238	71. 566 60. 419 29. 856 1. 00 11. 79 A	C
ATOM	1710	CD1 TYR	238	71. 451 59. 139 29. 317 1. 00 16. 12 A	C
ATOM	1711	CE1 TYR	238	70. 292 58. 739 28. 635 1. 00 17. 09 A	C
ATOM ATOM	1712 1713	CD2 TYR CE2 TYR	238 238	70. 496 61. 295 29. 701 1. 00 12. 13 A 69. 336 60. 913 29. 020 1. 00 12. 94 A	C
ATOM	1714	CZ TYR	238		C C
VI OIII	1114	OL III	400	69. 243 59. 634 28. 487 1. 00 15. 48 A	U

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					FI	G. 4	- 36			(Continued)
						U .				
ATOM	1715	OH	TYR	238	68. 127	59. 257	27.775	1.00 15.96	Α	0
ATOM	1716	C	TYR	238	74. 445	59.847	28. 954	1.00 15.25	Α	С
ATOM	1717	0	TYR	238	74. 059	59.667	27. 798	1.00 17.74	A	0
ATOM	1718	N	SER	239	75. 220	58. 986	29. 596	1.00 14.10	A	Ŋ
ATOM	1719	CA	SER	239	75. 689	57.779	28. 943	1.00 13.87	A	Ç
ATOM	1720	CB	SER	239	76. 926	57. 251	29.656	1.00 11.90	A	C
ATOM	1721	0G	SER	239	77. 902	58. 265	29. 766	1.00 18.76	A	0
ATOM	1722	C	SER	239	74.661	56.668		1.00 13.45	A	C
ATOM	1723	0	SER	239	73. 755	56. 587	29.700	1.00 14.39	A	0
ATOM	1724	N	PHE	240	74.809	55.834		1.00 12.12	A	N
ATOM	1725	CA	PHE	240	73. 972	54.678		1.00 12.95	A	C
ATOM	1726	CB	PHE	240	73.003	54. 833		1.00 12.48	A	C
ATOM	1727	CG	PHE	240	71.896	53.843		1.00 11.50	A	C
ATOM	1728		PHE	240	70.824	54.037		1.00 10.15	A	C
ATOM	1729		PHE	240	71.980	52.655	25.858	1.00 11.95	A	C
ATOM	1730		PHE	240	69. 859	53.064		1.00 10.78	A	C
ATOM	1731		PHE	240	71.018	51.675		1.00 11.03	A	C
ATOM	1732	CZ	PHE	240	69. 954	51.878		1.00 10.46	A	C
ATOM	1733	C	PHE	240	75.018	53. 652		1.00 14.83	A	C
ATOM	1734	0	PHE	240	75. 722	53. 805	26. 335	1.00 18.18	A	0
ATOM	1735	N	TYR	241	75. 129	52. 617		1.00 13.74	A	N
ATOM	1736	CA	TYR	241	76.147	51.612	27. 958	1.00 13.29	A	C
ATOM	1737	CB	TYR	241	76. 526	51.057	29. 329	1.00 13.69	A	C
ATOM	1738	CG	TYR	241	76.833	52. 167	30. 317	1.00 10.88	A	C
ATOM	1739		TYR	241	78.065	52. 821	30. 308	1.00 11.93	A	C
ATOM	1740		TYR	241	78. 326	53. 894		1.00 9.47	A	C
ATOM	1741		TYR	241	75. 862	52.610		1.00 12.15	A	C
ATOM	1742		TYR	241	76. 106	53. 678		1.00 11.02	A	C
ATOM	1743	CZ	TYR	241	77. 338	54. 319		1.00 12.15	A	C
ATOM	1744	0H	TYR	241	77. 556	55. 408		1.00 10.38	A	0
ATOM	1745	C	TYR	241	75. 793	50.510		1.00 14.62	. A	C
ATOM	1746	0 N	TYR	241	76. 686	49. 948		1.00 12.20	· A	0 N
ATOM	1747	N	SER SER	242	74. 501	50. 204		1.00 16.13	A	N C
ATOM	1748	CA		242	74.053	49. 180		1.00 16.13	A	
ATOM ATOM	1749	CB	SER SER	242	74. 464	49.590		1.00 16.30	A	C
ATOM	1750	OG C	SER	242	74.004	48.674		1.00 17.85	A	0 C
ATOM	1751 1752		SER	242	74.647	47. 816 47. 625	27. 303	1.00 17.46 1.00 19.13	A	0
ATOM	1753	O N	ASP	242	75. 219 74. 516	46. 865	25. 312	1.00 19.13	A A	N N
ATOM	1754		ASP	243	75. 066	45. 535	25. 548	1.00 13.34	A	C
ATOM	1755	CA CB	ASP	243	74. 774	44. 605	24. 369	1.00 23.30	A	Č
ATOM	1756	CG	ASP	243	73. 290	44. 419	24. 309	1.00 27.30	A	C
ATOM	1757		ASP	243 243	72. 549	44. 246	25. 126	1.00 35.83	A	0
ATOM	1758		ASP	243 243	72. 862	44. 438	22. 955	1.00 30.37	A	0
ATOM	1759	C	ASP	243 243	76. 572	45. 554		1.00 37.13	A	Č
ATOM	1760	0	ASP	243 243	77. 298	46. 432	25. 330	1.00 23.30	A	Ŏ
ATOM	1761	N	GLU	243 244	77. 016	44. 559	26. 567	1.00 24.45	A	N
ATOM	1762	CA	GLU	244	78. 412	44. 363		1.00 22.80	A	Č
ATOM	1763	CB	GLU	244	78. 534	42. 984		1.00 23.73	A	č

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ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	1778 (1779 (1780 (1781 (1782 (1783 (1784 N1785 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (1786 (CB CCD1 CCD2 C C O V CA CB	LEU LEU LEU LEU LEU GLN GLN GLN	246 246 246 246 246 246 247 247 247	78. 594 78. 522 78. 659 78. 736 77. 458 80. 943 80. 921 82. 034 83. 295 84. 400	48. 926 50. 368 50. 388 51. 181 48. 463 48. 662 48. 635 49. 073 49. 038	23. 229 22. 728	1.00 18.41 1.00 18.20 1.00 17.99 1.00 16.83 1.00 19.98 1.00 18.12 1.00 16.81 1.00 17.84 1.00 17.30 1.00 15.11	A A A A A A A	C C C C C O N C C	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	1788 C 1789 C 1790 N 1791 C 1792 C 1793 N 1794 C	VE2 C)	GLN GLN GLN GLN GLN TYR TYR TYR	247 247 247 247 247 247 248 248 248	85. 791 86. 875 86. 829 87. 862 83. 224 83. 640 82. 710 82. 592	49. 234 48. 770 49. 065 48. 049 50. 461 50. 648 51. 436 52. 794	23. 045 22. 090 20. 899 22. 611 24. 170 25. 313 23. 430 23. 954	1.00 17.62 1.00 18.47 1.00 20.53 1.00 17.76 1.00 17.66 1.00 17.56 1.00 18.50 1.00 19.00	A A A A A A	C C O N C O N C	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	1796 C 1797 C 1798 C 1799 C 1800 C 1801 C	CG CD1 CD2 CD2 CE2 CZ CH	TYR	248 248 248 248 248 248 248 248 248	83. 177 84. 684 85. 353 86. 742 85. 444 86. 839 87. 479 88. 854 81. 130	53. 822 53. 820 52. 812 52. 814 54. 838 54. 851 53. 836 53. 809 53. 134	22. 972 22. 860 22. 172 22. 058 23. 437 23. 333 22. 647 22. 595 24. 212	1.00 17.39 1.00 16.80 1.00 17.20 1.00 17.58 1.00 17.77 1.00 17.22 1.00 18.42 1.00 19.27 1.00 18.87	A A A A A A	000000000	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	1804 0 1805 N 1806 C 1807 C 1808 C 1809 C 1810 C 1811 0 1812 N	D A B G	TYR PRO PRO PRO PRO PRO PRO PRO PRO LYS	248 249 249 249 249 249 249 249 249	80. 288 80. 804 81. 610 79. 411 79. 424 80. 857 78. 937 79. 734 77. 638	53. 018 53. 549 53. 595 53. 886 54. 222 54. 582 55. 042 55. 864 55. 096	23. 323 25. 440 26. 668 25. 716 27. 206 27. 481 24. 852 24. 413 24. 599	1.00 19.15 1.00 18.20 1.00 18.21 1.00 18.83 1.00 19.46 1.00 17.63 1.00 19.66 1.00 20.92 1.00 19.01	A A A A A A A	0 N C C C C C O N	

			FIG. 4-38							
ATOM	1813 CA L	YS 250	77.083 56.158 23.785 1.00 19.61	A C						
ATOM		YS 250	75. 933 55. 618 22. 936 1. 00 23. 51	A C						
ATOM		YS 250	76. 320 54. 428 22. 089 1. 00 28. 40	A C						
ATOM		YS 250	75. 197 54. 010 21. 152 1. 00 30. 62	A C						
ATOM		YS 250	75.698 52.938 20.203 1.00 32.02	A C						
ATOM		YS 250	76. 966 53. 385 19. 546 1. 00 32. 62	A N						
ATOM		YS 250	76.580 57.320 24.628 1.00 17.92	A C						
ATOM	1820 0 L	YS 250	76.130 57.130 25.758 1.00 17.90	A 0						
ATOM		HR 251	76.663 58.524 24.077 1.00 14.61	A N						
ATOM		HR 251	76.171 59.689 24.786 1.00 15.48	A C						
ATOM		HR 251	77. 104 60. 887 24. 666 1. 00 13. 61	A C						
ATOM		THR 251	78. 280 60. 654 25. 441 1. 00 15. 96	A 0						
ATOM	1825 CG2 T		76. 414 62. 137 25. 181 1. 00 13. 93	A C						
ATOM		HR 251	74. 832 60. 086 24. 205 1. 00 16. 04	A C						
ATOM		HR 251	74. 755 60. 572 23. 083 1. 00 17. 34	A 0						
ATOM		AL 252	73. 779 59. 860 24. 977 1. 00 15. 27	A N						
ATOM		AL 252	72. 439 60. 205 24. 559 1. 00 16. 08	A C						
ATOM		AL 252	71. 405 59. 381 25. 355 1. 00 16. 76	A C						
ATOM	1831 CG1 V		69. 987 59. 832 25. 014 1. 00 16. 29	A C						
ATOM	1832 CG2 V		71.595 57.895 25.050 1.00 13.65	A C						
ATOM		AL 252	72. 223 61. 699 24. 799 1. 00 18. 46 72. 443 62. 212 25. 905 1. 00 19. 01	A C A 0						
ATOM		/AL 252	72. 443 62. 212 25. 905 1. 00 19. 01 71. 799 62. 398 23. 754 1. 00 19. 18	A N						
ATOM		ARG 253 ARG 253	71. 568 63. 831 23. 842 1. 00 18. 54	A C						
ATOM ATOM		IRG 253	72.574 64.567 22.949 1.00 19.46	A C						
ATOM		RG 253	74.014 64.439 23.457 1.00 24.49	A C						
ATOM		ARG 253	75.021 65.066 22.519 1.00 29.04	A C						
ATOM		ARG 253	75. 797 64. 044 21. 822 1. 00 35. 89	A N						
ATOM		ARG 253	77. 013 63. 647 22. 185 1. 00 38. 08	A C						
ATOM	1842 NH1 A		77. 606 64. 191 23. 241 1. 00 39. 69	A N						
ATOM	1843 NH2 A		77. 633 62. 699 21. 497 1. 00 40. 12	A N						
ATOM		ARG 253	70.140 64.156 23.449 1.00 17.33	A C						
ATOM		ARG 253	69.690 63.802 22.362 1.00 18.44	A 0						
ATOM		/AL 254	69.432 64.836 24.344 1.00 16.85	A N						
ATOM		/AL 254	68.033 65.196 24.125 1.00 15.67	A C						
ATOM	1848 CB V	/AL 254	67.079 64.405 25.070 1.00 16.67	A C						
ATOM	1849 CG1 V	/AL 254	65.640 64.775 24.766 1.00 16.79	A C						
ATOM	1850 CG2 V	/AL 254	67. 308 62. 899 24. 951 1. 00 17. 24	A C						
ATOM		/AL 254	67. 737 66. 660 24. 405 1. 00 14. 62	A C						
ATOM		/AL 254	68. 122 67. 186 25. 450 1. 00 15. 12	A 0						
ATOM		PRO 255	67. 048 67. 340 23. 475 1. 00 13. 71	A N						
ATOM		PRO 255	66. 677 66. 945 22. 105 1. 00 10. 62	A C						
ATOM		PRO 255	66. 725 68. 749 23. 730 1. 00 13. 00	A C						
ATOM		PRO 255	66. 064 69. 193 22. 431 1. 00 13. 28	A C						
ATOM		PRO 255	66. 674 68. 265 21. 397 1. 00 13. 45	A C						
ATOM		PRO 255	65. 735 68. 674 24. 899 1. 00 13. 86	A C						
ATOM		PRO 255	64.663 68.086 24.772 1.00 13.58	A 0						
ATOM		TYR 256	66. 108 69. 255 26. 032 1. 00 13. 63	A N A C						
ATOM	1861 CA 7	TYR 256	65.304 69.194 27.242 1.00 11.65	n U						

				(Continued)
			FIG. 4-39	(COLULTION)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	1866 CD: 1867 CE: 1868 CZ 1869 OH 1870 C 1871 O 1872 N 1873 CD 1874 CA 1875 CB 1876 CG 1877 C 1878 O 1879 N 1880 CA 1881 CB	1 TYR 25 2 TYR 25 2 TYR 25 TYR 25 TYR 25 TYR 25 TYR 25 TYR 25 PRO 25	65. 801 68. 006 28. 077 1. 00 10. 57 A 65. 044 67. 706 29. 351 1. 00 10. 49 A 64. 949 68. 646 30. 378 1. 00 9. 61 A 64. 296 68. 351 31. 571 1. 00 7. 54 A 64. 460 66. 460 29. 549 1. 00 9. 65 A 63. 799 66. 156 30. 735 1. 00 11. 05 A 63. 722 67. 105 31. 742 1. 00 10. 10 A 63. 060 66. 801 32. 909 1. 00 10. 49 A 65. 488 70. 492 28. 012 1. 00 12. 70 A 66. 559 70. 750 28. 553 1. 00 12. 70 A 64. 444 71. 325 28. 080 1. 00 12. 39 A 63. 174 71. 254 27. 334 1. 00 13. 82 A 64. 548 72. 593 28. 800 1. 00 11. 47 A 63. 501 73. 450 28. 106 1. 00 12. 01 A 62. 405 72. 464 27. 866 1. 00 12. 87 A 64. 296 72. 489 30. 298 1. 00 12. 85 A 65. 327 72. 718 31. 105 1. 00 11. 64 A 65. 155 72. 671 32. 546 1. 00 11. 10 A 66. 501 72. 439 33. 227 1. 00 12. 96	
ATOM ATOM ATOM	1882 CG 1883 CD 1884 CE	LYS 25 LYS 25 LYS 25	67. 034 71. 012 33. 031 1. 00 14. 20 A 68. 519 70. 906 33. 331 1. 00 13. 34 A 69. 042 69. 480 33. 136 1. 00 13. 95 A	C C C
ATOM ATOM ATOM ATOM ATOM	1885 NZ 1886 C 1887 O 1888 N 1889 CA	LYS 25 LYS 25 LYS 25 ALA 25 ALA 25	64. 517 73. 984 33. 011 1. 00 12. 44 A 64. 368 74. 921 32. 224 1. 00 11. 13 A 64. 124 74. 043 34. 280 1. 00 13. 33 A	. C . O . N
ATOM ATOM ATOM ATOM	1890 CB 1891 C 1892 O 1893 N	ALA 25 ALA 25 ALA 25 GLY 26	63. 368 75. 097 36. 355 1. 00 16. 40 A 64. 167 76. 555 34. 508 1. 00 15. 14 A 65. 317 76. 787 34. 881 1. 00 17. 32 A 63. 448 77. 419 33. 802 1. 00 16. 82 A	C C C O N
ATOM ATOM ATOM ATOM ATOM	1894 CA 1895 C 1896 O 1897 N 1898 CA	GLY 26 GLY 26 GLY 26 ALA 26 ALA 26	64. 870 78. 749 32. 217 1. 00 15. 78 A 65. 379 79. 812 31. 852 1. 00 17. 65 A 65. 072 77. 600 31. 577 1. 00 13. 77 A	C O N
ATOM ATOM ATOM ATOM	1899 CB 1900 C 1901 O 1902 N	ALA 26 ALA 26 ALA 26 VAL 26	66. 524 76. 182 30. 224 1. 00 10. 21 A 65. 093 77. 911 29. 137 1. 00 10. 04 A 63. 896 78. 160 29. 212 1. 00 8. 71 A 65. 747 77. 947 27. 987 1. 00 11. 73 A	C C O N
ATOM ATOM ATOM ATOM ATOM ATOM		VAL 26 VAL 26 I VAL 26 VAL 26 VAL 26 VAL 26	66.035 78.529 25.594 1.00 11.50 A 65.257 78.796 24.299 1.00 8.31 A 66.939 79.732 25.920 1.00 5.79 A 64.092 77.167 26.389 1.00 13.92 A	C ···· C C
ATOM ATOM	1909 N 1910 CA	ASN 263 ASN 263	62.844 77.536 26.139 1.00 13.49 A	N

										(Continued)
					FΙ	G. 4	- 40			(00
ATOM	1911	CB	ASN	263	60.470	77.038	26.336	1.00 14.53	Α	С
ATOM	1912	CG	ASN	263	60. 222		27.746	1.00 17.27	Α	C
ATOM	1913		ASN	263	59. 342		28.444	1.00 18.62	Α	0
ATOM	1914		ASN	263	60.977		28. 169	1.00 16.78	A	Ň
		C	ASN	263	61. 715		24. 265	1.00 14.45	A	Ċ
MOTA	1915				62. 170		23. 561	1.00 14.43		ŏ
ATOM	1916	0	ASN	263					A	
ATOM	1917	N	PRO	264	61.119		23. 743	1.00 14.86	A	N
ATOM	1918	CD	PR0	264	60. 513		24. 412	1.00 15.86	Ą	C
ATOM	1919	CA	PR0	264	60. 986		22. 294	1.00 15.41	A	C
ATOM	1920	CB	PR0	264	60. 591	73.844	22.106	1.00 14.97	A	C
ATOM	1921	CG	PR0	264	59. 721	73.607	23.287	1.00 14.81	Α	С
ATOM	1922	C	PR0	264	59. 867	76.238	21.882	1.00 15.66	Α	C
ATOM	1923	0	PR0	264	58. 954	76.496	22.663	1.00 17.42	Α	0
ATOM	1924	N	THR	265	59.942		20.673	1.00 15.76	Α	N
ATOM	1925	CA	THR	265	58. 895		20.199	1.00 14.67	Α	C
ATOM	1926	CB	THR	265	59. 458		19.341	1.00 15.37	A	Č
ATOM	1927	0G1		265	60. 162		18. 223	1.00 15.98	A	Ö
ATOM	1928	CG2		265	60. 402		20. 159	1.00 12.01	A	č
ATOM	1929	C	THR	265	58. 024		19.360	1.00 15.62	A	č
										Ŏ
ATOM	1930	0 N	THR	265	58. 465		18. 932	1.00 18.75	A	
ATOM	1931	N	VAL	266	56. 794		19.113	1.00 15.56	A	N
ATOM	1932	CA	VAL	266	55. 872		18. 347	1.00 12.79	A	C
ATOM	1933	CB	VAL	266	54. 856		19. 274	1.00 12.90	A	C
ATOM	1934	CG1		266	54. 193		20. 130	1.00 12.06	A	C
ATOM	1935		VAL	266	53. 821	74.920	18.466	1.00 10.69	A	C
ATOM	1936	C	VAL	266	55. 115		17. 350	1.00 12.88	A	C
ATOM	1937	0	VAL	266	54. 995		17.511	1.00 12.12	Α	0
ATOM	1938	N	LYS	267	54.601	76.501	16.327	1.00 13.52	Α	N
ATOM	1939	CA	LYS	267	53.817	77. 107	15. 262	1.00 13.08	Α	C
ATOM	1940	CB	LYS	267	54. 692	77. 389	14.050	1.00 13.64	Α	C
ATOM	1941	CG	LYS	267	55. 642	78.570	14.165	1.00 13.17	Α	C
ATOM	1942	CD	LYS	267	56. 348		12.833	1.00 11.33	Α	C
ATOM	1943	CE	LYS	267	57. 313		12.788	1.00 11.66	Ā	Ċ
ATOM	1944	NZ	LYS	267	58. 007		11.459	1.00 12.98	Ā	N
ATOM	1945	C	LYS	267	52. 713		14.851	1.00 14.81	A	Ċ
ATOM	1946	ŏ	LYS	267	52. 885		14. 930	1.00 14.01	A	ŏ
ATOM	1947	N	PHE	268	51. 588		14. 389	1.00 14.31	A	N
ATOM	1948	CA	PHE	268	50. 471		13. 975	1.00 13.02	A	Č
										C
ATOM	1949	CB	PHE	268	49. 249		14.842	1.00 13.98	A	C
ATOM	1950	CG	PHE	268	48. 237		14.846	1.00 15.65	A	C
ATOM	1951		PHE	268	48. 467		15. 562	1.00 15.51	A	C
ATOM	1952		PHE	268	47. 056		14. 115	1.00 18.05	A	C
ATOM	1953		PHE	268	47. 537		15.551	1.00 15.17	A	C
ATOM	1954		PHE	268	46. 120		14. 101	1.00 17.28	A	C
ATOM	1955	CZ	PHE	268	46. 366		14. 821	1.00 14.54	A	C
ATOM	1956	C	PHE	268	50.117		12. 497	1.00 14.63	Α	С
ATOM	1957	0	PHE	268	50.143		11.981	1.00 16.53	Α	0
ATOM	1958	N	PHE	269	49. 767		11.829	1.00 13.37	Α	N
ATOM	1959	CA	PHE	269	49.417		10.413	1.00 12.73	Α	С

					F I	G. 4	- 41			(Continued)
ATOM	1960				50. 597	74. 510	9.547	1.00 12.68	Α	С
ATOM	1961	CG			51.875		9.809		Α	Ċ
ATOM	1962		1 PHE		52. 190		9.112		A	Č
ATOM	1963		2 PHE		52.758		10.770	1.00 11.04	A	C
ATOM	1964		1 PHE		53. 374			1.00 12.54	Α	C
ATOM	1965		2 PHE		53.940				Α	C
ATOM	1966	CZ			54. 252			1.00 13.89	Α	C
ATOM	1967	Ç	PHE		48. 270				Α	C
ATOM	1968		PHE		47. 937			1.00 14.50	Α	0
ATOM	1969	N	VAL		47.699				Α	N
ATOM	1970	CA			46.626			1.00 15.44	Α	C
ATOM	1971	CB	VAL		45. 228			1.00 14.59	Α	C
ATOM	1972		1 VAL		44. 153			1.00 12.94	A	С
ATOM	1973		2 VAL		45. 110			1.00 15.69	Α	С
ATOM ATOM	1974 1975	C	VAL		46. 730			1.00 16.91	A	C
ATOM	1976	O N	VAL VAL		46. 875	74. 188		1.00 17.51	A	0
ATOM	1977	CA	VAL	271 271	46. 681	71.966		1.00 17.37	A	N
ATOM	1978	CB	VAL	271	46. 726	71.746		1.00 16.54	A	C
ATOM	1979		VAL	271	47. 928 47. 911	70.879		1.00 19.07	A	C
ATOM	1980		VAL.	271	47. 878	69. 548		1.00 20.07	A	C
ATOM	1981	C	VAL	271	45. 456	70. 635 71. 041	3. 131	1.00 18.62	A	C
ATOM	1982	ŏ	VAL	271	44.912	70. 226	4. 641 5. 383	1.00 15.09 1.00 13.46	A	C
ATOM	1983	Ň	ASN	272	44. 988	71. 394	3. 449	1.00 15.40	A	0 N
ATOM	1984	CA	ASN	272	43. 812	70. 802	2. 832	1.00 13.17	A A	N
ATOM	1985	CB	ASN	272	43. 231	71. 767	1. 797	1.00 13.83	A	C C
ATOM	1986	CG	ASN	272	42.010	71. 205	1.093	1.00 14.46	A	Č
ATOM	1987		ASN	272	41.822	69.989	1.007	1.00 16.67	A	Ö
ATOM	1988		ASN	272	41.175	72.090	0.581	1.00 15.74	Ä	Ň
ATOM	1989	C	ASN	272	44.310	69. 542	2.110	1.00 15.70	Ä	Ĉ
ATOM	1990	0	ASN	272	44. 755	69.617	0.967	1.00 16.88	A	Ö
ATOM	1991	N	THR	273	44. 241	68.390	2.758	1.00 15.93	A	N
ATOM	1992	CA	THR	273	44.717	67. 169	2.124	1.00 18.97	Α	C
ATOM	1993	CB	THR	273	44.570	65.936	3.052	1.00 19.44	Α	C
ATOM	1994	001	THR	273	43. 201	65. 794	3.471	1.00 19.69	Α	0
ATOM ATOM	1995		THR	273	45. 481	66.083	4. 266	1.00 19.20	Α	С
ATOM	1996 1997	C	THR	273	44.009	66.870	0.813	1.00 19.92	A	C
ATOM	1998	0 N	THR	273	44. 550	66. 154	-0.028	1.00 21.20	Ą	0
ATOM	1999	CA	ASP ASP	274	42.811	67. 424	0.634	1.00 20.50	A	N
ATOM	2000	CB	ASP	274 274	42.032	67. 193	-0.584	1.00 20.30	Ą	C
ATOM	2001	CG	ASP	274	40.578	67. 629	-0.390	1.00 21.02	A	C
ATOM	2001		ASP	274 274	39. 705 38. 543	66. 529	0.178	1.00 23.48	A	C
ATOM	2002		ASP	274	40. 168	66. 823 65. 375	0.527	1.00 26.38	A	0
ATOM	2004	C	ASP	274	42. 573	65. 375 67. 870	0. 275 -1. 832	1.00 23.88	A	0
ATOM	2005	ŏ	ASP	274	42. 131	67. 556	-1.832 -2.932	1.00 19.89	A	C .
ATOM	2006	Ň	SER	275	43. 508	68. 802	-2. 932 · -1. 676	1. 00 22. 08 1. 00 18. 13	A	0 N
ATOM	2007	CA	SER	275	44. 073	69. 490	-2. 834	1.00 18.13	A A	N C
ATOM	2008	CB	SER	275	44. 284	70.969	-2.518	1.00 19.37	A	Č .

			٠.	F I G. 4 - 42	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2020 2021 2022 2023 2024 2025 2026 2027 2028 2029 2030 2031 2032 2033 2034 2035 2036 2037 2038 2039 2040	OG SE O SE O SE O SE CA LE CG LE CCD1 LE CCD2 LE CCD2 LE CCD3 SE CCD3 SE CCD4 SE CCD5 SE CCD6 SE CCD7 SE CCCD7 SE CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	RR 275 RR 276 UU 276 UU 276 UU 276 276 276 276 276 277 277 RR 277 RR 277 RR 277 RR 278 RR 279 LL 279 LL 279 LL 279 LL 279 LL 279 LL 279 RR 280	45. 197 71. 121 -1. 444 1. 00 24. 82 45. 397 68. 885 -3. 314 1. 00 19. 53 45. 883 69. 226 -4. 394 1. 00 19. 59 45. 971 67. 986 -2. 516 1. 00 19. 83 47. 241 67. 348 -2. 846 1. 00 20. 72 47. 545 66. 226 -1. 849 1. 00 19. 96 47. 725 66. 641 -0. 392 1. 00 20. 47 47. 991 65. 410 0. 456 1. 00 21. 68 48. 875 67. 622 -0. 277 1. 00 18. 56 47. 360 66. 790 -4. 263 1. 00 22. 34 48. 290 67. 137 -4. 994 1. 00 24. 63 46. 434 65. 925 -4. 656 1. 00 22. 80 46. 501 65. 325 -5. 983 1. 00 23. 82 45. 456 64. 219 -6. 121 1. 00 23. 44 46. 305 66. 341 -7. 097 1. 00 24. 47 46. 699 66. 104 -8. 231 1. 00 26. 86 45. 698 67. 472 -6. 768 1. 00 25. 44 45. 431 68. 522 -7. 745 1. 00 26. 20 44. 051 69. 121 -7. 471 1. 00 25. 70 43. 831 70. 266 -8. 266 1. 00 30. 53 46. 495 69. 630 -7. 739 1. 00 25. 70 48. 327 70. 696 -6. 672 1. 00 26. 01 48. 327 70. 696 -6. 565 1. 00 28. 42 48. 073 71. 634 -5. 350 1. 00 29. 96 49. 372 72. 211 -4. 834 1. 00 32. 19 47. 148 72. 768 -5. 776 1. 00 29. 90 49. 704 70. 043 -6. 470 1. 00 28. 21 49. 834 68. 872 -6. 088 1. 00 29. 00 A 50. 728 70. 801 -6. 848 1. 00 26. 67 A 52. 092 70. 306 -6. 832 1. 00 26. 53	
ATOM ATOM ATOM ATOM ATOM	2042 2043 2044 2045 2046	OG1 THI CG2 THI C THI O THI N ASI	R 280 R 280 R 280 R 280 V 281	52. 533 71. 331 -8. 986 1. 00 29. 98 A 54. 422 70. 645 -7. 674 1. 00 26. 85 A 52. 618 70. 254 -5. 418 1. 00 26. 01 A 53. 184 69. 255 -4. 986 1. 00 27. 33 A 52. 402 71. 341 -4. 696 1. 00 25. 17 A	C O C C O N
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2048 (2049 (2050 (2051 12052 (2053 (2054 12055 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (2056 (CA ASI CB ASI CG ASI OD1 ASI ND2 ASI C ASI O ASI N ALA CA ALA C ALA	N 281 N 281 N 281 N 281 N 281 N 281 N 281 N 282 A 282	52. 876 71. 474 -3. 334 1. 00 23. 78 A 54. 190 72. 250 -3. 388 1. 00 22. 28 A 54. 925 72. 287 -2. 071 1. 00 22. 87 A 54. 603 71. 576 -1. 116 1. 00 20. 83 A 55. 948 73. 136 -2. 056 1. 00 22. 18 A 51. 818 72. 211 -2. 506 1. 00 23. 12 A 51. 876 73. 431 -2. 362 1. 00 22. 47 A 50. 849 71. 460 -1. 982 1. 00 23. 33 A 49. 763 72. 018 -1. 166 1. 00 23. 40 A 48. 952 70. 895 -0. 547 1. 00 23. 19 A 50. 320 72. 912 -0. 071 1. 00 24. 45 A	C C C O N C O N C C C

				,						(Continued)
					FΙ	G. 4	- 43			(OUIIIIIII)
ATOM	2058	0	ALA		51.180	72. 487	0.694	1.00 25.49	A	0
ATOM	2059	N	THR		49.817	74. 140	0.024	1.00 24.70	A	Ŋ
ATOM	2060	CA	THR		50. 326	75.074	1.021	1.00 25.33	A	C
ATOM	2061	CB	THR		50. 209	76. 540	0.539		. A	C
ATOM	2062	0G1			48. 834	76.874	0.353	1.00 29.84	A	0
ATOM	2063	CG2			50.947	76. 730	-0. 785	1.00 30.06	A	C
ATOM	2064	C	THR		49.710	74. 983	2.406	1.00 24.49	A	C
ATOM	2065	0	THR		48. 487	74. 960	2.578	1.00 24.13	A	0
ATOM	2066	N	SER		50. 593	74.941	3.396	1.00 23.17	A	N
ATOM ATOM	2067 2068	CA	SER		50. 200	74.872	4. 791	1.00 19.88	A	C
ATOM	2000	CB OG	SER SER		51.317	74. 249	5.624	1.00 15.88	A	C
ATOM	2009	C	SER		51.413 49.906	72. 868 76. 275	5. 350 5. 288	1.00 14.23 1.00 19.24	A	0
ATOM	2071	0	SER		50. 774	77. 148	5. 253	1.00 19.24	A	C 0
ATOM	2072	N	ILE	285	48. 674	76. 478	5. 745	1.00 13.03	A A	N
ATOM	2073	CA	ILE	285	48. 249	77. 771	6. 242	1.00 17.30	A	C
ATOM	2074	CB	ILE	285	46. 754	78. 003	5.977	1.00 16.10	A	Č
ATOM	2075		ILE	285	46. 384	79. 446	6.324	1.00 10.55	A	Č
ATOM	2076		ILE	285	46. 434	77. 691	4.513	1.00 14.89	A	Č
ATOM	2077	CD1		285	47. 230	78. 526	3. 528	1.00 15.03	A	č
ATOM	2078	C	ILE	285	48. 496	77. 848	7. 733	1.00 16.46	Ä	č
ATOM	2079	Ō	ILE	285	48. 116	76. 963	8. 489	1.00 18.69	A	ŏ
ATOM	2080	N	GLN	286	49. 130	78. 923	8. 159	1.00 16.66	A	Ň
ATOM	2081	CA	GLN	286	49. 428	79.088	9.563	1.00 16.43	Ä	Ċ
ATOM	2082	CB	GLN	286	50.778	79.776	9.717	1.00 16.31	Ā	Č
ATOM	2083	CG	GLN	286	51.184	80.070	11.135	1.00 17.85	Ā	Č
ATOM	2084	CD	GLN	286	52.552	80.713	11.196	1.00 21.44	Α	C
ATOM	2085		GLN	286	53.072	81.005	12.277	1.00 24.09	Α	0
ATOM	2086		GLN	286	53. 149	80. 939	10.028	1.00 19.13	Α	N
ATOM	2087	C	GLN	286	48. 360	79. 885	10. 289	1.00 16.82	Α	C
ATOM	2088	0	GLN	286	47. 794	80.844	9.754	1.00 17.23	Α	0
ATOM	2089	N	ILE	287	48.070	79. 453		1.00 15.99	Α	N
ATOM	2090	CA	ILE	287	47. 116	80. 137	12.355	1.00 15.11	A	C
ATOM	2091	CB	ILE	287	46. 036			1.00 14.14	A	Č
ATOM	2092		ILE	287	45.147	79. 916	13.875	1.00 14.36	A	C
ATOM	2093		ILE	287	45. 206	78. 621	11.742	1.00 13.29	A	C
ATOM	2094		ILE	287	44.111	77.675	12. 202	1.00 14.31	A	C
ATOM ATOM	2095 2096	C	ILE	287	47. 991	80.625	13.506	1.00 15.35	A	C
ATOM	2090	0 N	ILE	287	48.349	79, 860	14.401	1.00 14.39	A	0
ATOM	2098		THR THR	288	48. 367	81.894	13, 452	1.00 15.01	A	N
ATOM	2098	CA CB		288	49. 215	82. 465	14. 482	1.00 16.71	A	C
ATOM	2100	OG1	THR THR	288 288	49. 688 48. 548	83.874	14.093	1.00 17.36	A	C
ATOM	2100	CG2		288	50.621	84. 679 83. 813	13. 779 12. 881	1.00 21.17 1.00 17.64	A	0
ATOM	2102	CGZ	THR	288	48.510	82. 553	15.818	1.00 17.04	A A	C ·
ATOM	2102	0	THR	288	47. 287	82.668	15. 888	1.00 16.02	A	0
ATOM	2104	N	ALA	289	49. 301	82. 488	16. 881	1.00 16.25	A	N N
ATOM	2105	CA	ALA	289	48. 787	82. 582	18. 232	1.00 16.67	A	C
ATOM	2106	CB	ALA	289	49. 887	82. 262	19. 207	1.00 18.89	A	Č
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F I G. 4 - 44											
ATOM ATOM ATOM	2107 2108 2109	C O N	ALA ALA PRO	289 289 290	48. 280 48. 629	84. 001 84. 927 84. 193	18. 467 17. 733 19. 487	1.00 18.05 1.00 19.12 1.00 18.60	A A A	C O N	
ATOM ATOM	2110 2111	CD CA	PRO PRO	290 290	46. 851 46. 906	83. 189 85. 526	20. 388 19. 783	1.00 18.37 1.00 19.04	A A	C	
ATOM ATOM ATOM	2112 2113 2114	CB CG	PRO PRO PRO	290 290 290	46.306	85. 234 84. 055 86. 447	20. 777 21. 499 20. 369	1.00 17.58 1.00 19.78 1.00 20.45	A A A	C C C	
ATOM ATOM ATOM	2115 2116 2117	O N CA	PRO ALA ALA	290 291 291	47.878	85. 995 87. 735 88. 728	21. 092 20. 054 20. 543	1.00 22.14 1.00 19.85 1.00 19.27	A A A	O N C	
ATOM ATOM	2118 2119	CB C	ALA ALA	291 291	48. 330 49. 101	90. 132 88. 610	20. 213 22. 041 22. 489	1.00 17.30 1.00 19.66 1.00 21.52	A A	C C	
ATOM ATOM ATOM	2120 2121 2122	O N CA	ALA SER SER	291 292 292	48. 074 48. 275	88. 791 88. 305 88. 185	22. 825 24. 264	1.00 19.16 1.00 19.97	A A A	O N C	
ATOM ATOM ATOM	2123 2124 2125	CB OG C	SER SER SER	292 292 292	46. 259 49. 244	87. 983 86. 839 87. 055	24. 971 24. 487 24. 618	1.00 19.90 1.00 24.94 1.00 20.24	A A A	C O C	
ATOM ATOM ATOM	2126 2127 2128	O N CA	SER MET MET	292 293 293	49.566	86. 948 86. 214 85. 104	25. 760 23. 635 23. 818	1.00 21.86 1.00 20.06 1.00 18.78	A A A	O N C	
ATOM ATOM ATOM	2129 2130 2131	CB CG SD	MET MET MET	293 293 293	49. 987 48. 795	83. 830 83. 168 82. 503	23. 149 23. 797 25. 424	1.00 17.35 1.00 15.90 1.00 15.89	A A A	C C S	
ATOM ATOM ATOM	2132 2133 2134	CE C	MET MET MET	293 293 293	47.655 51.831	82. 993 85. 487	26. 296 23. 161	1.00 16.41 1.00 20.24	A A	C C	
ATOM ATOM	2135 2136	N CA	LEU LEU	294 294	51. 738 52. 918	85. 221 86. 116 86. 532	23. 693 21. 995 21. 255	1.00 21.12 1.00 20.44 1.00 21.31	A A A	O N C	
ATOM ATOM ATOM	2137 2138 2139		LEU LEU LEU	294 294 294	51.850	87. 104 86. 092 86. 820	19. 900 18. 944 17. 747	1.00 21.19 1.00 23.63 1.00 22.60	A A A	C C	
ATOM ATOM ATOM	2140 2141 2142	CD2 C O	LEU LEU LEU	294 294 294	53.818		18. 493 21. 981 21. 564	1.00 20.94 1.00 22.05 1.00 23.39	A A A	C C 0	
ATOM ATOM ATOM	2143 2144 2145	N CA CB	ILE ILE ILE	295 295 295	53. 329 54. 149	88. 156 89. 122 89. 938	23. 053 23. 792 24. 835	1.00 21.86 1.00 22.24 1.00 24.92	A A A	N C C	
ATOM ATOM ATOM	2146 2147 2148	CG2 CG1	ILE ILE ILE	295 295 295	52. 084 52. 906	90. 536 89. 034 89. 761	24. 196 25. 998 27. 085	1.00 25.08 1.00 25.57 1.00 26.45	A A A	C C C	
ATOM ATOM	2149 2150	C 0	ILE ILE	295 295	55. 271 56. 218	88. 426 89. 064	24. 565 25. 006	1.00 21.97 1.00 23.91	A A	C 0	
ATOM ATOM ATOM	2151 2152 2153	N CA C	GLY GLY GLY	296 296 296	56. 174 56. 165	87. 119 86. 401 84. 922	24. 749 25. 482 25. 167	1.00 20.65 1.00 18.90 1.00 18.45	A A A	N C C	
ATOM ATOM	2154 2155	O N	GLY ASP	296 297		84. 503 84. 132	24. 202 25. 967	1.00 18.61 1.00 16.58	A A	O N	

										(Con	tinued)
					FΙ	G. 4	- 45			(00-	
ATOM ATOM ATOM ATOM	2156 2157 2158 2159		ASP ASP ASP	297 297 297 297	56. 918 57. 960 59. 366 59. 553	82. 694 82. 032 82. 378 82. 882	25. 751 26. 650 26. 253 25. 128	1.00 16.95 1.00 18.00 1.00 18.62 1.00 18.23	A A A	C C C	
ATOM ATOM ATOM ATOM	2160 2161 2162 2163	C O N	ASP ASP ASP HIS	297 297 297 298	60. 284 55. 553 54. 847 55. 190	82. 134 82. 096 82. 537 81. 079	27. 063 26. 041 26. 942 25. 279	1.00 21.29 1.00 16.02 1.00 16.36 1.00 14.79	A A A	0 C 0 N	
ATOM ATOM ATOM	2164 2165 2166	CA CB CG	HIS HIS HIS	298 298 298	53. 901 52. 846 53. 245	80. 449 81. 207 81. 448	25. 460 24. 661 23. 241	1.00 16.82 1.00 14.81 1.00 15.31	A A A	C C C	
ATOM ATOM ATOM ATOM	2167 2168 2169 2170	ND1 CE1	HIS HIS HIS	298 298 298 298	52. 921 54. 127 54. 327 53. 608	80. 793 82. 442 82. 392 81. 400	22. 099 22. 876 21. 572 21. 076	1.00 14.85 1.00 13.01 1.00 14.39 1.00 14.38	A A A	C N C N	
ATOM ATOM ATOM	2171 2172 2173	C O N	HIS HIS TYR	298 298 299	53. 956 55. 008 52. 802	79. 008 78. 519 78. 348	24. 979 24. 560 25. 031	1.00 17.54 1.00 15.53 1.00 17.25	A A A	C O N	
ATOM ATOM ATOM ATOM	2174 2175 2176 2177	CA CB CG CD1	TYR TYR TYR TYR	299 299 299 299	52. 675 52. 666 53. 811 55. 095	76. 963 76. 029 76. 176 75. 762	24. 609 25. 816 26. 790 26. 456	1.00 16.58 1.00 15.77 1.00 17.03 1.00 14.29	A A A	C C C	
ATOM ATOM ATOM ATOM	2178 2179 2180 2181		TYR TYR TYR TYR	299 299 299 299	56. 119 53. 586 54. 600 55. 865	75. 807 76. 653 76. 700 76. 270	27. 380 28. 081 29. 009 28. 656	1.00 15.79 1.00 15.17 1.00 15.67 1.00 15.90	A A A	C C C	
ATOM ATOM ATOM	2182 2183 2184	0 C OĤ	TYR TYR TYR	299 299 299	56. 863 51. 351 50. 349	76. 261 76. 741 77. 411	29. 595 23. 893 24. 178	1.00 16.73 1.00 17.76 1.00 16.87	A A A	0 C 0	
ATOM ATOM ATOM ATOM	2185 2186 2187 2188	N CA CB CG	LEU LEU LEU LEU	300 300 300 300	51. 355 50. 130 50. 413 49. 232	75. 799 75. 413 74. 923 74. 296	22. 959 22. 292 20. 878 20. 139	1.00 16.20 1.00 16.36 1.00 16.40 1.00 14.78	A A A	N C C C	
ATOM ATOM ATOM	2189 2190 2191	CD1 CD2 C	LEU LEU LEU	300 300 300	48. 131 49. 692 49. 777	75. 322 73. 789 74. 243	19. 972 18. 785 23. 205	1.00 16.55 1.00 15.08 1.00 17.58	A A A	C C C	
ATOM ATOM ATOM ATOM	2193 2194	O N CA CB	LEU CYS CYS CYS	300 301 301 301	50. 568 48. 629 48. 288 48. 208	73. 312 74. 290 73. 202 73. 722	23. 335 23. 873 24. 782 26. 220	1.00 17.21 1.00 19.46 1.00 22.20 1.00 22.63	A A A	O N C C	
ATOM ATOM	2198	SG C O	CYS CYS CYS	301 301 301	46. 943 47. 032 46. 690	74. 962 72. 399 71. 481	26. 503 24. 468 25. 210	1.00 26.56 1.00 23.29 1.00 25.66	A A A	S C O	
ATOM ATOM ATOM ATOM	2200 2201	N CA CB CG	ASP ASP ASP ASP	302 302 302 302	46. 341 45. 148 43. 999 42. 789	72. 731 71. 976 72. 223 71. 355	23. 386 23. 015 23. 991 23. 680	1.00 23.55 1.00 24.19 1.00 26.49 1.00 28.68	A A A	N C C C	
ATOM ATOM	2203	0D1 0D2	ASP	302 302	42. 795 41. 841	70. 170 71. 844	24. 066 23. 029	1.00 30.65 1.00 30.37	A A	0 0	

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(Continued) FIG. 4-46 C 72.292 21.610 1.00 23.22 ATOM 2205 C ASP 302 44.658 0 73.455 21.226 1.00 24.26 2206 **ASP** 302 44.523 A ATOM 0 44.385 N 71.237 20.857 1.00 21.65 A 2207 VAL 303 ATOM N 43.902 71.349 19.493 1.00 20.79 C 303 A 2208 VAL ATOM CA C 70.803 18.480 1.00 21.88 44.926 CB VAL 303 Α ATOM 2209 Ċ 17.051 44.420 71.028 1.00 20.34 A **ATOM** 2210 CG1 VAL 303 C **ATOM** 2211 CG2 VAL 303 46.273 71.465 18.702 1.00 20.12 A 303 42.657 70.494 19.417 1.00 20.38 A C 2212 **ATOM** C VAL 69.306 19.744 1.00 19.45 0 303 42.687 A 2213 VAL **ATOM** 0 71.102 18.982 1.00 20.04 N 41.562 A 304 **ATOM** 2214 N THR C 40.302 70.394 18.882 1.00 19.30 A **ATOM** 2215 CA THR 304 C 39.494 70.546 20.191 1.00 19.73 **ATOM** 2216 CB THR 304 A 0 OG1 THR 304 40.256 70.024 21.287 1.00 20.19 A **ATOM** 2217 38.168 69.812 20.090 1.00 17.51 C 304 A ATOM 2218 CG2 THR C 39.467 70.930 17.733 1.00 18.56 2219 304 A ATOM THR C 72.127 17.674 0 39.185 1.00 19.32 304 **ATOM** 2220 0 THR 70.042 16.819 1.00 18.08 N **ATOM** 2221 N TRP 305 39.082 A C ATOM 2222 CATRP 305 38.243 70.422 15.681 1.00 16.88 A 2223 TRP 305 38.332 69.394 14.546 1.00 13.92 A C ATOM CB 39.581 69.464 13.745 1.00 13.82 C TRP 2224 CG 305 A ATOM C 12.606 1.00 13.04 CD2 TRP 305 39.815 70.296 A 2225 **ATOM** 70.068 C 12.189 305 41.143 1.00 13.12 **ATOM** 2226 CE2 TRP A 39.031 71.216 11.899 C **ATOM** 2227 CE3 TRP 305 1.00 13.55 A 68. 781 C **ATOM** 2228 CD1 TRP 305 40.745 13.967 1.00 13.51 A NE1 TRP 305 41.688 69.138 13.036 1.00 11.41 A N 2229 ATOM 305 41.704 70.729 11.094 C **ATOM** 2230 CZ2 TRP 1.00 12.03 Α 2231 39.591 10.809 CZ3 TRP 305 71.873 1.00 14.16 C **ATOM** A C 71.625 40.914 10.419 1.00 13.92 **ATOM** 2232 CH2 TRP 305 A 2233 C TRP 305 36.803 70.477 16.155 1.00 16.35 C ATOM 69.613 1.00 16.55 ATOM 2234 0 TRP 305 36.368 16.917 A 0 2235 306 36.064 71.484 15.704 1.00 16.10 ATOM N **ALA** N 71.620 2236 ALA 306 34.661 16.079 1.00 17.20 A C ATOM CA 34.336 73.074 16.384 1.00 18.47 A C ATOM 2237 CB ALA 306 33.770 C ATOM 2238 C ALA 306 71.110 14.956 1.00 16.79 A ATOM 2239 306 32.829 70.369 15.191 1.00 18.46 0 0 ALA A **ATOM** 2240 N THR 307 34.076 71.516 13.733 1.00 18.36 A N 2241 CA 33.314 71.100 12.564 1.00 18.83 C **ATOM** THR 307 A 2242 307 32.387 72.222 12.072 1.00 18.43 C ATOM CB THR A 33.178 73.254 11.473 2243 0G1 THR 307 1.00 20.76 **ATOM** A 0 **ATOM** 2244 CG2 THR 307 31.593 72.811 13.225 1.00 16.72 A C 34.299 C ATOM 307 70.778 11.442 1.00 20.34 2245 C THR A **ATOM** 2246 0 THR 307 35.494 70.626 11.689 1.00 22.05 0 A 2247 GLN 308 33.798 70.688 10.213 1.00 20.11 N N **ATOM** A 1.00 19.71 34.640 2248 CA GLN 308 70.389 9.066 C **ATOM** A 2249 1.00 19.44 **ATOM** CB GLN 308 33.799 69.942 7.866 A C 2250 CG GLN 308 32.845 68.791 8.118 1.00 21.53 C ATOM 33.524 1.00 23.81 CD 308 67.505 8.557 C ATOM 2251 GLN A 66.565 OE1 GLN 308 32.854 9.003 1.00 25.80 A 0 2252 ATOM

SUBSTITUTE SHEET (RULE 26)

67.449

8.430

1.00 21.04

N

34.848

2253

ATOM

NE2 GLN

308

					FIC	G. 4	- 47				(Con	tinued)
ATOM	2254	С	GLN	308	35. 440	71.616	8. 653	1 00	19. 98	٨	ſ	
ATOM	2255	Ö	GLN	308	36. 421	71. 501	7. 922		21.84	A	C	
ATOM	2256	N	GLU	309	35. 022	72. 789	9.114		19.41	A	0	
ATOM	2257	CA	GLU	309	35. 710	74. 019	9. 114 8. 751		20. 93	A	N	
ATOM	2258	CB	GLU	309		74. 764	7. 685		21.98	A	C	
ATOM	2259	CG	GLU	309		73. 971	6.419		26. 38	A	C C	
ATOM	2260	CD	GLU	309		74. 731	5. 413	1.00		A	C	
ATOM	2261	0E1		309		74. 192	4. 305		31.98	A A	0	
ATOM	2262		GLU	309		75. 869	5. 736		28. 78	A	0	
ATOM	2263	C	GLU	309		74. 939	9. 932	1.00		A	C	
ATOM	2264	ŏ	GLU	309		76. 152	9. 764	1.00		A	0	
ATOM	2265	Ň	ARG	310		74. 360	11.125	1.00		A	N	
ATOM	2266	CA	ARG	310		75. 131	12. 340	1.00		A	Č	
ATOM	2267	CB	ARG	310		75. 445	12.986	1.00		A	Č	
ATOM	2268	CG	ARG	310		76. 186	14. 305	1.00		A	Č	
ATOM	2269	CD	ARG	310		76. 630	14. 786	1.00		A	Č	
ATOM	2270	NE	ARG	310		77. 605	13.870	1.00		A	N	
ATOM	2271	CZ	ARG	310		77. 884	13. 785	1.00		Ä	Ĉ	
ATOM	2272	NH1	ARG	310		77. 261	14. 569	1.00		Ä	Ň	
ATOM	2273	NH2	ARG	310		78. 776	12.902	1.00		A	N	
ATOM	2274	C	ARG	310		74. 346	13.304	1.00		Ä	Ċ	
ATOM	2275	0	ARG	310		73. 214	13.671	1.00		Ä	Ö	
ATOM	2276	N	ILE	311	38. 108	74. 959	13.710	1.00		Α	N	
ATOM	2277	CA	ILE	311		74.320	14.619	1.00	17.41	Α	C	
ATOM	2278	CB	ILE	311		73. 991	13.859	1.00		Α	C	
ATOM	2279		ILE	311		75. 252	13.305	1.00		A	C	
ATOM	2280	CG1		311		73. 254	14.765	1.00		Α	C	
ATOM	2281	CD1		311	42.589	72. 763	14.011	1.00		A	C	
ATOM	2282	C	ILE	311		75. 258	15.802	1.00		A	C	
ATOM	2283	0	ILE	311		76. 481	15.649	1.00		Α	0	
ATOM ATOM	2284 2285	N	SER	312		74. 692	16.988	1.00		A	N	
ATOM	2286	CA	SER	312		75.517	18. 163	1.00		A	C	
ATOM	2287	CB OG	SER SER	312 312		75. 244	19. 235	1.00		A	C	
ATOM	2288	C	SER	312		74. 173	20.074	1.00		A	0	
ATOM	2289	0	SER	312		75. 269 74. 131	18. 736	1.00		A	C	
ATOM	2290	N	LEU	313		76. 349	18. 795 19. 148	1.00		A	0	
ATOM	2291	CA	LEU	313		76. 271	19. 708	1.00 1 1.00 2		A	N	
ATOM	2292	CB	LEU	313		76. 931	18. 768	1.00 1		A	C	
ATOM	2293	ĊĞ	LEU	313		76. 409	17. 341	1.00		A	C	
ATOM	2294		LEU	313		77. 038	16. 712	1.00 1		A A	C C	
ATOM	2295		LEU	313		74. 892	17. 351	1.00 2			C	
ATOM	2296	C	LEU	313		76. 957	21.062	1.00 2		A A	C	
ATOM	2297	Ŏ	LEU	313		78. 030	21. 265	1.00 2		A	0	
ATOM	2298	Ň	GLN	314		6. 333	21. 981	1.00 2		· A	N	
ATOM	2299	CA	GLN	314		6. 884	23. 308	1.00 2		A	C	
ATOM	2300	CB	GLN	314		5. 935	24. 365	1.00 2		Ä	Č	
ATOM	2301	CG	GLN	314		5. 860	24. 406	1.00 2		Ä	č	
ATOM	2302	CD	GLN	314		4. 832	25. 401	1.00 2		Ä	č	

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					FΙ	G. 4	- 48			(0022022000	-7
ATOM	2303	ሰ ፑ1	GLN	314	A1 097	74. 911	26. 598	1.00 29.38	٨		.•
ATOM	2304		GLN	314	41.827 40.786	73. 854	24. 911	1.00 29.30	A A	O N	
ATOM	2305	C	GLN	314	45. 584	77. 099	23. 532	1.00 30.32	A	C	
ATOM	2306	ő	GLN	314	46. 382	76. 176	23. 419	1.00 22.34	A	Ö	
ATOM	2307	N	TRP	315	45. 954	78. 333	23. 833	1.00 21.50	A	N	
ATOM	2308	CA	TRP	315	47. 343	78. 667	24. 070	1.00 20.70	A	C	
ATOM	2309	CB	TRP	315	47. 748	79. 873	23. 226	1.00 18.74	Ä	Č	
ATOM	2310	ĊĠ	TRP	315	47. 480	79. 711	21.746	1.00 17.87	Ä	č	
ATOM	2311		TRP	315	48. 435	79. 368	20. 733	1.00 14.81	Ä	Č	
ATOM	2312		TRP	315	47.764	79.419	19.491	1.00 14.29	Ä	Č	
ATOM	2313	CE3	TRP	315	49. 793	79.029	20.753	1.00 13.32	Α	C	
ATOM	2314	CD1	TRP	315	46. 299	79.936	21.095	1.00 15.84	Α	С	
ATOM	2315		TRP	315	46.463	79. 769	19.742	1.00 13.87	Α	N	
ATOM	2316		TRP	315	48. 407	79. 147	18. 278	1.00 12.51	Α	С	
ATOM	2317		TRP	315	50. 433	78. 760	19.545	1.00 13.87	A	C	
ATOM	2318		TRP	315	49. 736	78.822	18.325	1.00 12.57	Α	C	
ATOM	2319	C	TRP	315	47. 530	78.976	25. 545	1.00 21.60	Α	C	
ATOM	2320	0	TRP	315	46. 615	79. 463	26. 205	1.00 22.41	A	0	
ATOM	2321	N	LEU	316	48. 721	78. 689	26.056	1.00 21.81	A	N	
ATOM	2322	CA	LEU	316	49.033	78. 915	27. 458	1.00 22.64	A	C	
ATOM	2323	CB	LEU	316	49.034	77. 573	28. 192	1.00 22.20	A	C	
ATOM	2324	CG	LEU	316	49.655	77. 484	29. 584	1.00 23.04	A	C	
ATOM ATOM	$\begin{array}{c} 2325 \\ 2326 \end{array}$		LEU	316	48. 953	78. 438	30. 530	1.00 24.08	A	C	
ATOM	2327	CDZ	LEU LEU	316 316	49.557	76.049	30.085	1.00 19.71	A	C	
ATOM	2328	Õ	LEU	316	50. 383 51. 392	79. 617 79. 192	27. 618 27. 046	1.00 24.44 1.00 26.77	A	C	
ATOM	2329	N	ARG	317	50. 388	80. 704	28. 383	1.00 20.77	A	O N	
ATOM	2330	CA	ARG	317	51.603	81. 475	28. 630	1.00 23.52	A A	C	
ATOM	2331	CB	ARG	317	51. 265	82. 787	29. 337	1.00 25.72	A	C	
ATOM	2332	CG	ARG	317	50. 490	83. 785	28. 504	1.00 26.72	A	C	
ATOM	2333	CD	ARG	317	50. 187	85. 012	29. 327	1.00 26.99	A	Č	
ATOM	2334	NE	ARG	317	49. 796	86. 141	28. 494	1.00 30.37	A	N	
ATOM	2335	CZ	ARG	317	49. 278	87. 269	28. 966	1.00 30.55	A	č	
ATOM	2336		ARG	317	49.082	87.414	30. 273	1.00 29.99	Ā	Ň	
ATOM	2337	NH2	ARG	317	48.972	88. 256	28.132	1.00 28.53	A	N	
ATOM	2338	C	ARG	317	52. 580	80.705	29.500	1.00 21.07	Α	C	
ATOM	2339	0	ARG	317	52.175	79.920	30. 359	1.00 19.79	Α	0	
ATOM	2340	N	ARG	318	53. 871	80. 941	29. 290	1.00 19.43	Α	N	
ATOM	2341	CA	ARG	318	54.876	80. 259	30.084	1.00 17.08	Α	С	
ATOM	2342	CB	ARG	318	56. 263	80.850	29.845	1.00 15.15	Α	C	
ATOM	2343	CG	ARG	318	57. 345	80.075	30. 564	1.00 13.58	Ą	C	
ATOM	2344	CD	ARG	318	58.671	80.165	29.853	1.00 13.59	A	C	
ATOM	2345	NE	ARG	318	59.687	79. 341	30. 504	1.00 11.13	A	Ŋ	
ATOM	2346	CZ	ARG	318	60.895	79. 135	30.001	1.00 10.46	A	Ç	
ATOM	2347	NH1	ARG	318	61.220	79.694	28. 850	1.00 11.29	A	N	
ATOM ATOM	2348 2349		ARG	318	61.773	78. 378	30. 642	1.00 10.86	A	N	
ATOM	2349	C 0	ARG	318	54. 500 54. 704	80.354	31.555	1.00 16.61	A	C	
ATOM	2351	N N	ARG ILE	318	54. 794	79.448	32. 318	1.00 20.33	A	0 N	
VION	4001	11	ILC	319	53. 869	81.455	31.954	1.00 16.59	A	N	

•										(Continued)
					FΙ	G. 4	- 49			
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2352 2353 2354 2355 2356 2357 2358 2359 2360 2361 2362	CG1 CD1 C O N CA CB CG	ILE ILE ILE ILE ILE ILE ILE ILE GLN GLN GLN	319 319 319 319 319 319 320 320 320 320	53. 396 53. 389 52. 720 54. 828 55. 712 51. 972 51. 870 50. 623 50. 939 52. 000	81. 607 83. 078 83. 210 83. 589 82. 743 81. 065 81. 808 79. 747 79. 001 77. 516 77. 044	33. 330 33. 776 35. 128 33. 878 34. 787 33. 251 33. 067 33. 381 33. 246 33. 420 32. 444	1. 00 17. 40 1. 00 17. 03 1. 00 17. 19 1. 00 19. 57 1. 00 19. 56 1. 00 17. 56 1. 00 18. 71 1. 00 16. 94 1. 00 16. 12 1. 00 14. 59 1. 00 12. 17	A A A A A A A A	C C C C C C C C C
ATOM ATOM ATOM	2363 2364 2365		GLN	320 320 320	52. 304 51. 431 53. 554	75. 577 74. 734 75. 261	32. 570 32. 403 32. 860	1.00 10.79 1.00 12.70 1.00 13.71	A A A	C O N
ATOM ATOM ATOM ATOM	2366 2367 2368 2369	C O N CA	GLN GLN ASN ASN	320 320 321 321	49. 368 48. 645 49. 079	79. 351 78. 466 80. 633 81. 010	34. 038 34. 472 34. 207	1. 00 16. 32 1. 00 14. 51 1. 00 18. 37 1. 00 19. 38	A A A	C O N
ATOM ATOM ATOM	2370 2371 2372	CB CG	ASN ASN ASN	321 321 321 321	47. 871 48. 226 48. 776 49. 166	81. 785 83. 166 83. 491	34. 931 36. 203 35. 925 34. 804	1. 00 19. 38 1. 00 20. 21 1. 00 23. 59 1. 00 22. 35	A A A	C C C 0
ATOM ATOM ATOM	2373 2374 2375		ASN ASN ASN	321 321 321	48. 801 46. 983 46. 095	83. 975 81. 843 82. 555	36. 980 34. 020 34. 479	1. 00 27. 82 1. 00 18. 69 1. 00 19. 10	A A A	N C O
ATOM ATOM ATOM	2376 2377 2378	N CA CB	TYR TYR TYR	322 322 322	47. 222 46. 482 47. 105	81. 715 82. 466 83. 856	32. 719 31. 719 31. 599	1.00 17.65 1.00 18.28 1.00 18.09	A A A	N C C
ATOM ATOM ATOM ATOM	2379 2380 2381 2382	CE1	TYR TYR TYR TYR	322 322 322 322	46. 319 46. 561 45. 843 45. 340	84. 856 85. 037 85. 987 85. 645	30. 792 29. 428 28. 694 31. 401	1.00 20.14 1.00 21.33 1.00 22.14 1.00 20.00	A A A	C C C C
ATOM ATOM ATOM	2383 2384 2385		TYR TYR TYR	322 322 322 322	44. 624 44. 876 44. 163	86. 589 86. 758 87. 704	30. 681 29. 334 28. 638	1.00 20.00 1.00 19.18 1.00 21.74 1.00 24.04	A A A	C C O
ATOM ATOM ATOM	2386 2387 2388	C O N	TYR TYR SER	322 322 323	46. 518 47. 583 45. 351	81. 750 81. 587 81. 318	30. 363 29. 764 29. 896	1.00 18.70 1.00 18.36 1.00 17.43	A A A	C O N
ATOM ATOM ATOM	2389 2390 2391	CA CB OG	SER SER SER	323 323 323	45. 237 44. 871 43. 662	80. 638 79. 163 79. 025	28. 612 28. 806 29. 535	1. 00 17. 45 1. 00 16. 45 1. 00 17. 51	A A A	C C O
ATOM ATOM ATOM ATOM	2392 2393 2394 2395	C O N CA	SER SER VAL VAL	323 323 324 324	44. 163 43. 250 44. 277 43. 309	81. 320 81. 943 81. 199 81. 802	27. 777 28. 314 26. 461 25. 555	1.00 17.88 1.00 18.20 1.00 18.44 1.00 18.83	A A A	C O N C
ATOM ATOM ATOM ATOM	2396 2397 2398	CB CG1 CG2	VAL VAL	324 324 324 324	43. 925 42. 944 44. 290	82. 995 83. 509 84. 105	24. 800 23. 760 25. 785	1.00 19.32 1.00 18.46 1.00 18.78	A A A	C C C
ATOM ATOM	2399 2400	C 0	VAL VAL	324 324	42. 839 43. 631	80. 776 79. 985	24. 534 24. 036	1. 00 18. 47 1. 00 18. 75	A A	C 0

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(Continued) FIG. 4-50 N **ATOM** 2401 325 80.772 24.231 N MET 41.5491.00 17.55 **ATOM** 2402 CA MET 325 41.046 79.832 23.245 1.00 17.68 C A 39.832 **ATOM** 2403 CBMET 325 79.062 23.769 1.00 19.82 C Α **ATOM** 2404 CG MET 325 39.272 78.043 22.774 1.00 20.18 C A 23.268 SD MET 325 37.681 77.304 1.00 23.11 S **ATOM** 2405 Α \mathbf{c} 38.209 ATOM 2406 CE MET 325 75.734 23.896 1.00 24.95 A 325 C 21.999 2407 MET 40.641 80.584 1.00 18.03 C ATOM Α 22.076 1.00 16.88 **ATOM** 2408 0 MET 325 39.932 81.583 A 0 ATOM 2409 ASP 326 41.114 80.118 20.852 N 1.00 18.60 N A **ATOM** CA ASP 326 40.749 80.738 19.595 1.00 20.69 2410 Α C 41.988 18.797 C **ATOM** 2411 CB ASP 326 81.158 1.00 22.43 Α **ATOM** CG ASP 326 42.329 82.638 18.970 C 2412 1.00 26.03 Α OD1 ASP 19.547 41.511 83.384 **ATOM** 1.00 26.48 2413 326 A 0 ATOM 2414 OD2 ASP 326 43.415 83.063 18.518 1.00 28.75 A 0 39.924 79.739 **ATOM** 2415 C **ASP** 326 18.800 1.00 19.88 C Α **ATOM ASP** 40.254 78.563 18.729 2416 0 326 1.00 21.77 A 0 18. 223 327 38.832 80.208 1.00 20.27 **ATOM** 2417 N ILE N Α 37.980 17.419 **ATOM** 2418 CA ILE 327 79.355 1.00 22.22 A C C **ATOM** 2419 CB ILE 327 36.529 79.393 17.941 1.00 20.50 A **ATOM** 2420 CG2 ILE 327 35.600 78.697 16.985 1.00 19.07 \mathbf{c} A 19.305 327 36.483 **ATOM** 2421 CG1 ILE 78.691 1.00 21.51 C A **ATOM** 2422 CD1 ILE 327 35.164 78.766 20.006 1.00 20.97 Α 79.908 **ATOM** 2423 C ILE 327 38.113 16.015 1.00 23.66 C A 327 328 2424 80.984 **ATOM** 0 ILE 37.625 15.716 1.00 26.18 Α 0 CYS 38.804 2425 **ATOM** N 79.162 15.161 1.00 26.09 A N **ATOM** 2426 CA CYS 328 39.069 79.608 13.805 1.00 26.75 Α **ATOM** 2427 **CYS** 328 38.274 78.890 12.721 1.00 27.13 C Α 2428 CYS 328 38.168 77.663 **ATOM** 0 12.705 1.00 27.70 0 Α CYS 2429 CB 40.564 **ATOM** 328 79.481 13.547 1.00 27.02 A C SG CYS ATOM 2430 328 41.567 79.984 14.986 S 1.00 28.23 Α 37.729 ATOM 2431 N **ASP** 329 79.686 11.807 1.00 26.60 A N **ATOM** 2432 CA ASP 329 36.913 79.198 10.710 1.00 26.21 C Α **ATOM** 2433 CB ASP 35.595 79.969 10.690 329 1.00 24.92 Α C **ATOM** 2434 CG ASP 34.684 79.595 11.842 329 1.00 26.75 C Α **ATOM** 2435 OD1 ASP 329 35. 181 79.407 12.969 1.00 27.44 Α 0 79.493 **ATOM** 2436 OD2 ASP 329 33.460 11.625 1.00 28.96 Α 0 C ATOM 2437 **ASP** 329 37.613 79.349 9.367 1.00 28.54 Α C **ATOM** 2438 0 **ASP** 329 38.314 80.334 9.120 1.00 29.27 0 Α **ATOM** 2439 TYR N 330 37.416 78.371 8.492 1.00 29.31 Α N 78.411 **ATOM** 2440 CA TYR 330 38.027 7.173 1.00 29.64 C Α ATOM 2441 CB TYR 330 38.011 77.019 6.542 1.00 30.55 A C 38.597 **ATOM** 2442 330 CG TYR 76.980 5.151 1.00 31.78 C Α ATOM 2443 CD1 TYR 330 39.919 77.367 4.919 1.00 32.26 C A CE1 TYR 40.460 1.00 32.18 Č **ATOM** 2444 330 77.341 3.641 A CD2 TYR 330 37.832 76.561 1.00 32.94 **ATOM** 2445 4.066 A C CE2 TYR 330 38.364 76.526 1.00 32.62 C 2446 2.779 ATOM Α 330 39.676 1.00 33.67 ATOM 2447 CZ TYR 76.920 2.574 C Α TYR 330 1.00 34.33 2448 0H 40.193 76.914 1.299 ATOM Α 0 330 37.314 79.387 **ATOM** 2449 C TYR 6.243 1.00 30.14 C

					FIC	S. 4	- 51			(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2450 2451 2452 2453 2454 2455 2456 2457 2458 2461 2462 2463 2464 2465 2466 2467 2468 2469 2470 2471 2472 2473 2474 2475 2476 2477 2478 2477	OD2 C O N CA CB CG CD OE1	TYR ASP ASP ASP ASP ASP GLU GLU GLU GLU GLU GLU SER SER SER SER SER SER SER SER	330 331 331 331 331 331 332 332 332 332 332	36. 098 38. 074 37. 511 38. 191 37. 573 37. 570 37. 084 37. 750 38. 865 36. 690 36. 755 35. 388 35. 234 33. 869 33. 494 33. 175 37. 231 37. 846 36. 968 37. 388 36. 445 36. 669 38. 826 39. 324 39. 496 40. 883 40. 995 40. 954 41. 722	79. 313 80. 308 81. 262 82. 618 83. 661 83. 455 84. 684 80. 730 80. 170 77. 562 78. 970 77. 771 77. 534 80. 465 79. 982 81. 764 82. 652 83. 858 84. 795 83. 135 83. 163 84. 180 83. 536 81. 947 82. 029	6. 058 5. 666 4. 730 4. 862 3. 956 2. 724 4. 479 3. 336 2. 817	1. 00 28. 65 1. 00 31. 49 1. 00 33. 80 1. 00 36. 63 1. 00 39. 35 1. 00 40. 70 1. 00 42. 41 1. 00 35. 63 1. 00 36. 11 1. 00 37. 77 1. 00 38. 87 1. 00 43. 60 1. 00 47. 15 1. 00 48. 40 1. 00 38. 19 1. 00 38. 19 1. 00 39. 73 1. 00 37. 67 1. 00 38. 99 1. 00 38. 48 1. 00 40. 60 1. 00 37. 74 1. 00 38. 52 1. 00 38. 49 1. 00 37. 49 1. 00 38. 50 1. 00 38. 48 1. 00 35. 98 1. 00 36. 41	A A A A A A A A A A A A A A A A A A A	0 N C C C O O C C C O O C C O O C C O O C O O O C O O O O O O O O O O O O O O O O O O O O
ATOM ATOM	2480 2481	N CA	GLY GLY	335 335	41.064	32.029 30.817 79.620	1. 148 1. 263 1. 620	1.00 36.41 1.00 35.13 1.00 35.71	A A A	O N C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2482 2483 2484 2485 2486 2487 2488	C O N CA CB CG	GLY GLY ARG ARG ARG ARG ARG	335 335 336 336 336 336 336	42. 579 43. 574 442. 128 42. 783 43. 066 843. 957	79. 872 79. 201 80. 855 81. 197 82. 696 83. 232 84. 374	2. 894 3. 172 3. 666 4. 919 4. 991 3. 884 4. 416	1.00 35.19 1.00 35.61 1.00 33.99 1.00 33.15 1.00 36.78 1.00 42.04 1.00 45.76	A A A A A A	C O N C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2489 2490 2491 2492 2493 2494 2495	NE CZ	ARG ARG ARG	336 336 336 336 336 336 337	44. 010 8 44. 510 8 45. 805 8 43. 718 8 41. 935 8 40. 763 8	35. 359 36. 192 36. 159 37. 057 30. 801 30. 449 30. 869	5. 147 6. 055 6. 348 6. 675 6. 118 5. 981 7. 294	1. 00 48. 92 1. 00 50. 76 1. 00 52. 08 1. 00 52. 33 1. 00 30. 26 1. 00 29. 07 1. 00 26. 94	A A A A A	N C N N C O N
ATOM ATOM ATOM	2496 2497 2498	CA CB CG	TRP TRP TRP	337 337 337	41.869 8 42.616 7	30. 531 79. 403 78. 074	8. 533 9. 248 8. <u>561</u>	1. 00 24. 29 1. 00 19. 88 1. 00 15. 10	A A A	C C C

FIG. 4-52										(Continued)
АТОМ	2499	CDS	TRP	337	41.481	77.077	8. 861	1.00 9.80	A	С
ATOM			TRP	337	41.461	76. 026	7. 927	1.00 9.92	A	Č
ATOM ATOM	2500 2501		TRP	337	40.475	76. 970	9. 825	1.00 3.32	A	Č
ATOM	2502	CD1		337	43. 173	77. 601	7. 485	1.00 12.90	A	Č
ATOM	2502		TRP	337	42.688	76. 369	7. 099	1.00 9.82	A	N
ATOM	2504		TRP	337	40.849	74. 885	7. 935	1.00 9.71	A	Č
ATOM	2505		TRP	337	39.675	75. 836	9.832	1.00 7.79	Ä	č
ATOM	2506		TRP	337	39.866	74. 808	8.894	1.00 10.33	A	č
ATOM	2507	C	TRP	337	41.783	81. 758	9.425	1.00 24.55	Ä	Č
ATOM	2508	ŏ	TRP	337	42.794	82. 360	9.766	1.00 26.73	Ä	Ö
ATOM	2509	Ň	ASN	338		82. 128	9.806	1.00 25.00	A	N
ATOM	2510	CA	ASN	338	40.381	83. 296	10.648	1.00 26.17	Α	C
ATOM	2511	CB	ASN	338	39.464	84. 300	9.949	1.00 28.44	Α	C
ATOM	2512	CG	ASN	338	40.016	84. 761	8.612	1.00 30.42	Α	C
ATOM	2513	0D1	ASN	338	39. 320	84.711	7.596	1.00 32.04	Α	0
ATOM	2514	ND2	ASN	338	41.271	85. 217	8.606	1.00 28.33	Α	N
ATOM	2515	C	ASN	338		82.958	12.012	1.00 25.29	Α	C
ATOM	2516	0	ASN	338	38.957	82. 084	12.148	1.00 25.29	Α	0
ATOM	2517	N	CYS	339	40. 293	83.668	13.023	1.00 25.00	Α	N
ATOM	2518	CA	CYS	339	39.833	83. 482	14.389	1.00 24.73	A	C
ATOM	2519	C	CYS	339	39. 289	84. 829	14.888	1.00 22.42	A	Č
ATOM	2520	0	CYS	339	40.051	85. 717	15. 249	1.00 21.56	A	0
ATOM	2521	CB	CYS	339	40.992	83. 014	15. 285	1.00 25.93	A	C
ATOM	2522	SG	CYS	339	42.199	81.865	14.526	1.00 29.61	A	S
ATOM ATOM	2523 2524	N CA	LEU LEU	340 340	37. 968 37. 333	84. 978	14.889	1.00 22.38	A	N C
ATOM	2525	CB	LEU	340	35.839	86. 212 86. 185	15.347 15.069	1.00 20.83 1.00 19.89	A	C
ATOM	2526	CG	LEU	340	35. 364	86. 201	13.626	1.00 19.09	A A	C
ATOM	2527		LEU	340	33.877	85. 883	13.593	1.00 19.14	A	C
ATOM	2528		LEU	340	35.647	87. 551	13.012	1.00 19.00	A	C
ATOM	2529	C	LEU	340	37. 521	86. 406	16.835	1.00 20.16	Ä	č
ATOM	2530	ŏ	LEU	340	37. 337	85. 478	17.615	1.00 20.80	A	ŏ
ATOM	2531	Ň	VAL	341	37.866	87. 625	17. 225	1.00 20.46	Ä	Ň
ATOM	2532	CA	VAL	341				1.00 20.11	Ā	Č
ATOM	2533	CB	VAL	341		89. 399	18.786	1.00 21.45	Α	Ċ
ATOM	2534	CG1	VAL	341		89.647	20.221	1.00 22.38	Α	С
ATOM	2535	CG2	VAL	341	39.688	89.672	17.819	1.00 24.28	Α	C
ATOM	2536	C	VAL	341		87.749	19.403	1.00 18.51	Α	C
ATOM	2537	0	VAL	341		87. 423	20.585	1.00 17.77	A	0
ATOM	2538	N	ALA	342		87. 941	18. 731	1.00 19.68	Α	N
ATOM	2539	CA	ALA	342		87. 756	19.370	1.00 19.64	Ą	Č
ATOM	2540	CB	ALA	342		88. 125	18.407	1.00 18.89	A	C
ATOM	2541	C	ALA	342		86. 302	19.829	1.00 19.19	A	C
ATOM	2542	0	ALA	342		85. 987	20.580	1.00 18.12	A	0
ATOM	2543	N	ARG	343		85. 422	19.384	1.00 16.06	A	N
ATOM	2544	CA	ARG	343		84. 017	19.766	1.00 16.37	A	C
ATOM	2545 2546	CB CG	ARG	343			18.521	1.00 18.14	A	C
ATOM ATOM	2540 2547	CD	ARG ARG	343 343		83. 390 82. 695	17.687	1.00 20.31 1.00 21.82	A A	C C
AIUM	4041	ωU	UILU	040	აა. ისა	υ <i>α</i> . υσυ	10.00(1.00 41.04	. n	U

					FIG. 4-53	(Continued)
ATOM	2548	NE	ARG	343	32. 615 82. 969 15. 561 1. 00 23. 94 A	N
ATOM	2549		ARG	343	32. 373 82. 415 14. 383 1. 00 26. 14 A	Č
ATOM	2550	NH	1 ARG	343	33. 242 81. 559 13. 864 1. 00 28. 42 A	Ň
ATOM	2551	NH:	2 ARG	343	31. 256 82. 703 13. 734 1. 00 30. 23 A	N
ATOM	2552	C	ARG	343	36. 164 83. 603 20. 650 1. 00 17. 09 A	Ċ.
ATOM	2553	0	ARG	343	36. 275 82. 452 21. 057 1. 00 16. 76 A	0
ATOM	2554	N	GLN	344	37. 030 84. 553 20. 955 1. 00 18. 05 A	N
ATOM	2555	CA	GLN	344	38. 175 84. 267 21. 791 1. 00 18. 90 A	Ċ
ATOM	2556	CB	GLN	344	39. 191 85. 385 21. 645 1. 00 18. 03 A	Č
ATOM	2557	CG	GLN	344	40. 585 85. 012 22. 038 1. 00 17. 99 A	Ċ
ATOM	2558	CD	GLN	344	41.571 86.088 21.657 1.00 18.02 A	С
ATOM	2559		GLN	344	41.711 87.089 22.353 1.00 17.71 A	0
ATOM	2560		C GLN	344	42. 246 85. 897 20. 527 1. 00 17. 42 A	N
ATOM	2561	C	GLN	344	37. 708 84. 170 23. 234 1. 00 19. 61 A	С
ATOM	2562	0	GLN	344	37. 069 85. 087 23. 730 1. 00 21. 89 A	0
ATOM	2563	N	HIS	345	38. 013 83. 057 23. 897 1. 00 18. 47 A	N
ATOM	2564	CA	HIS	345	37. 624 82. 868 25. 287 1. 00 17. 92 A	C
ATOM	2565	CB	HIS	345	36. 786 81. 600 25. 453 1. 00 16. 07 A	C C C
ATOM ATOM	2566	CG	HIS	345	35. 478 81. 641 24. 726 1. 00 15. 01 A	C
ATOM	2567 2568		HIS	345	34. 223 81. 895 25. 164 1. 00 14. 43 A	C
ATOM	2569		HIS HIS	345	35. 371 81. 420 23. 369 1. 00 15. 56 A	N
ATOM	2570		HIS	$\frac{345}{345}$	34. 108 81. 535 23. 002 1. 00 12. 57 A	C
ATOM	2571	C	HIS	345	33. 390 81. 823 24. 073 1. 00 14. 20 A 38. 854 82. 789 26. 172 1. 00 19. 64 A	N
ATOM	2572	0	HIS	345	00 000	C
ATOM	2573	N	ILE	346	00 800 00 100	0
ATOM	2574	CA	ILE	346	00 000 00 701	N
ATOM	2575	CB	ILE	346	40 40# 04 000 00	C
ATOM	2576		ILE	346	14 000 01 000	C
ATOM	2577		ILE	346	10 000 05 000 05 55	C
ATOM	2578		ILE	346	40. 338 85. 860 27. 572 1. 00 19. 87 A 40. 466 87. 298 27. 978 1. 00 22. 20 A	C C
ATOM	2579	C	ILE	346	39. 657 82. 624 29. 482 1. 00 23. 76 A	Č
ATOM	2580	0	ILE	346	38. 535 82. 537 29. 975 1. 00 24. 67 A	0
ATOM	2581	N	GLU	347	40. 714 81. 976 29. 967 1. 00 25. 01 A	N N
ATOM	2582	CA	GLU	347	40. 601 81. 123 31. 141 1. 00 28. 30 A	Č
ATOM	2583	CB	GLU	347	40. 459 79. 656 30. 733 1. 00 26. 51 A	č
ATOM	2584	CG	GLU	347	40. 089 78. 740 31. 891 1. 00 27. 38 A	č
ATOM	2585	CD	GLU	347	40. 169 77. 268 31. 527 1. 00 29. 51 A	č
ATOM	2586		GLU	347	39. 877 76. 936 30. 359 1. 00 29. 48 A	ŏ
ATOM	2587		GLU	347	40. 511 76. 439 32. 405 1. 00 29. 57 A	Ö
ATOM	2588	C	GLU	347	41.836 81.288 32.021 1.00 30.87 A	Č
ATOM	2589	0	GLU	347	42. 865 80. 661 31. 777 1. 00 33. 35 A	Ō
ATOM	2590	N	MET	348	41.741 82.131 33.044 1.00 32.50 A	N
ATOM	2591	CA	MET	348	42. 877 82. 347 33. 926 1. 00 34. 46 A	C
ATOM	2592	CB	MET	348	43. 215 83. 843 34. 002 1. 00 37. 48 A	C
ATOM	2593	CG	MET	348	42. 168 84. 723 34. 661 1. 00 41. 62 A	С
ATOM	2594	SD	MET	348	42. 028 86. 340 33. 825 1. 00 48. 03 A	S
ATOM	2595	CE	MET	348	43. 541 87. 158 34. 341 1. 00 46. 60 A	С
ATOM	2596	С	MET	348	42. 628 81. 784 35. 315 1. 00 33. 55 A	С

					FIG. 4-54				
ATOM	2597	0	MET	348	41.656 81.070 35.541 1.00 34.35	Α	0		
ATOM	2598	Ň	SER	349	43.534 82.085 36.235 1.00 32.30	A	N		
ATOM	2599	CA	SER	349	43.428 81.623 37.612 1.00 31.26	A	C		
ATOM	2600	CB	SER	349	43. 961 80. 197 37. 744 1. 00 31. 22	A	C		
ATOM	2601	0G	SER	349	43.912 79.760 39.090 1.00 32.92	A	0		
ATOM	2602	C	SER	349	44. 244 82. 573 38. 474 1. 00 31. 16	A	Ç		
ATOM	2603	0	SER	349	45. 355 82. 950 38. 113 1. 00 31. 25	A	0		
ATOM	2604	N	THR	350	43. 682 82. 962 39. 611 1. 00 30. 83	A	N		
ATOM	2605	CA	THR	350	44.340 83.896 40.516 1.00 28.43	A	C		
ATOM	2606	CB	THR	350	43. 325 84. 938 41. 027 1. 00 28. 93	A	C		
ATOM	2607	0G1	THR	350	42. 251 84. 268 41. 703 1. 00 27. 68	A	0		
ATOM	2608	CG2		350	42.751 85.733 39.864 1.00 27.87	A	C		
ATOM	2609	C	THR	350	44. 971 83. 198 41. 714 1. 00 27. 14 45. 781 83. 786 42. 431 1. 00 27. 62	A	0 C		
ATOM	2610	0	THR	350	-	A A	N N		
ATOM	2611	N	THR	351 251	44.610 81.936 41.913 1.00 25.72 45.109 81.161 43.035 1.00 24.77	A	C		
ATOM	2612	CA CB	THR THR	351 351	43. 945 80. 536 43. 786 1. 00 25. 52	A	č		
ATOM ATOM	2613 2614	0G1	THR	351	43.166 79.746 42.877 1.00 24.95	A	ŏ		
ATOM	2615	CG2		351	43.069 81.617 44.385 1.00 24.61	A	Č		
ATOM	2616	C	THR	351	46.081 80.047 42.659 1.00 25.48	A	Č		
ATOM	2617	ŏ	THR	351	46.648 79.392 43.535 1.00 25.57	Ä	0		
ATOM	2618	Ň	GLY	352	46. 261 79. 825 41. 361 1. 00 25. 19	A	N .		
ATOM	2619	CA	GLY	352	47.170 78.786 40.909 1.00 24.62	A	C .		
ATOM	2620	C	GLY	352	47.371 78.797 39.403 1.00 24.61	A	C		
ATOM	2621	0	GLY	352	47.417 79.853 38.774 1.00 25.15	A	0		
ATOM	2622	N	TRP	353	47. 499 77. 612 38. 825 1. 00 23. 36	A	N		
ATOM	2623	CA	TRP	353	47.684 77.470 37.390 1.00 21.38	A	C		
ATOM	2624	CB	TRP	353	48. 631 76. 291 37. 116 1. 00 17. 49	A	C		
ATOM	2625	CG	TRP	353	48. 272 75. 023 37. 849 1. 00 16. 34	A	C		
ATOM	2626		TRP	353	48. 587 74. 693 39. 209 1. 00 14. 04	A	C		
ATOM	2627		TRP	353	48.053 73.409 39.462 1.00 14.33	A	C		
ATOM	2628		TRP	353	49. 270 75. 356 40. 238 1. 00 14. 55 47. 578 73. 957 37. 351 1. 00 14. 89	A	C		
ATOM	2629		TRP	353 353		A A	N N		
ATOM	2630 2631	(101 (79	TRP TRP	353	47. 445 72. 985 38. 311 1. 00 12. 84 48. 180 72. 768 40. 709 1. 00 14. 93	A	Č		
ATOM ATOM	2632		TRP	353	49.398 74.719 41.480 1.00 15.27	A	Č		
ATOM	2633		TRP	353	48. 853 73. 436 41. 700 1. 00 15. 07	Ä	C C C		
ATOM	2634	C	TRP	353	46. 303 77. 236 36. 782 1. 00 22. 43	A	Č		
ATOM	2635	ŏ	TRP	353	45. 307 77. 292 37. 495 1. 00 22. 69	Ä	Ō		
ATOM	2636	Ň	VAL	354	46. 231 76. 990 35. 479 1. 00 22. 83	A	N		
ATOM	2637	CA	VAL	354	44.944 76.749 34.836 1.00 24.15	A			
ATOM	2638	CB	VAL	354	44.818 77.513 33.498 1.00 25.09	Α	C		
ATOM	2639		VAL	354	43.610 77.006 32.718 1.00 24.29	A	C C C C		
ATOM	2640		VAL	354	44.673 79.007 33.762 1.00 24.71	A	C		
ATOM	2641	С	VAL	354	44. 799 75. 264 34. 569 1. 00 24. 96	A			
ATOM	2642	0	VAL		45.751 74.628 34.127 1.00 26.10	Ą	0		
ATOM	2643	N	GLY		43.609 74.722 34.841 1.00 24.28	A	N		
ATOM	2644	CA	GLY		43.354 73.303 34.640 1.00 22.67	A	C C		
ATOM	2645	C	GLY	355	44.040 72.457 35.696 1.00 22.77	A	U		

(Continued)

					FΙ	G. 4	- 55			(001
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2646 2647 2648 2649 2650 2651 2652 2653 2654 2655 2656 2657 2658 2660 2661 2662 2663	NH2 C O N CA CB CG CD1 CD2	GLY ARG ARG ARG ARG ARG ARG PHE PHE PHE PHE	355 356 356 356 356 356 356 356 356 357 357 357 357	44. 743 43. 843 44. 505 43. 927 42. 495 41. 973 40. 518 39. 849 40. 513 38. 520 45. 989 46. 844 46. 285 47. 659 48. 029 48. 173 49. 361 47. 126	72. 989 71. 145 70. 299 68. 886 68. 808 67. 391 67. 340 67. 607 67. 939 67. 547 70. 255 70. 508 69. 940 69. 876 68. 442 67. 524 67. 491 66. 693	36. 548 35. 668 36. 654 36. 645 37. 122 37. 036 37. 149 38. 261 39. 362 38. 272 36. 314 37. 163 35. 060 34. 587 34. 205 35. 380 36. 115 35. 763	1. 00 22. 56 1. 00 23. 29 1. 00 24. 86 1. 00 24. 91 1. 00 27. 84 1. 00 31. 58 1. 00 35. 53 1. 00 37. 59 1. 00 40. 39 1. 00 25. 60 1. 00 28. 06 1. 00 23. 61 1. 00 21. 95 1. 00 12. 89 1. 00 10. 46	A A A A A A A A A A A A A A A A A A A	
	2663 2664 2665 2666 2667 2668 2669 2670 2671 2672 2673 2674 2675 2676 2677 2678 2679 2680	CD2 CE1 CE2 CZ CO N CA CB CG CD NE CZ NH1					35. 763 37. 216 36. 863 37. 591 33. 377 33. 005 32. 782 31. 615 30. 396 30. 011 28. 598 28. 205 26. 943 25. 939 26. 687 31. 313 31. 734 30. 570	1.00 10.46		CCCCCONCCCCCNCNNCONCCCCCCO
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2687 2688 2689 2690 2691 2692 2693 2694	N CA CB OG C O N CA	SER SER SER SER SER SER GLU GLU	360 360 360 360 360 360 361 361	41. 499 40. 723 39. 501 38. 505 40. 262 40. 117 40. 024 39. 581	72. 350 71. 208 70. 986 71. 976 71. 280 72. 359 70. 104 69. 972	30. 070 29. 596 30. 497 30. 283 28. 140 27. 555 27. 573 26. 199	1. 00 22. 48 1. 00 24. 26 1. 00 25. 29 1. 00 27. 66 1. 00 25. 67 1. 00 25. 66 1. 00 27. 20	A A A A A A	N C C O C O N C

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					FΙ	G. 4	- 5 6			(Continued)
ATOM ATOM	2695 2696	CB CG	GLU GLU	361 361	39. 803 39. 356	68. 540 67. 444	25. 713 26. 683	1.00 30.37 1.00 36.42	A A	C C
ATOM	2697	CD	GLU		40.340	67. 226	27.839	1.00 30.42	A	Č
ATOM	2698		GLU	361	40. 317	68.002	28. 822	1.00 42.30	A	ő
ATOM	2699		GLU	361	41.152	66. 274	27.757	1.00 46.60	A	ŏ
ATOM	2700	Č	GLU	361	38. 112	70. 324	26.052	1.00 25.88	Ā	Č
ATOM	2701	Ŏ	GLU	361	37. 295	69.955	26. 888	1.00 27.12	Ā	0
ATOM	2702	N	PRO	362	37.760	71.061	24.989	1.00 23.97	Α	N
ATOM	2703	CD	PR0	362	38.650	71.837	24.106	1.00 23.33	Α	С
ATOM	2704	CA	PR0	362	36.365	71.436	24.767	1.00 22.45	Α	С
ATOM	2705	CB	PR0	362	36.485	72.714	23.945	1.00 23.21	Α	С
ATOM	2706	CG	PRO	362	37.679	72.437	23.100	1.00 21.08	Α	С
ATOM	2707	C	PR0	362	35. 621	70. 338	24.013	1.00 21.91	Α	C
ATOM	2708	0	PRO	362	36. 216	69. 582	23. 249	1.00 22.96	A	0
ATOM	2709	N	HIS	363	34. 318	70. 259	24. 245	1.00 21.59	A	Ŋ
ATOM	2710	CA	HIS	363	33. 459	69. 280	23. 596	1.00 19.88	A	C
ATOM	2711	CB	HIS	363	32. 868	68. 353	24. 649	1.00 18.03	A	C
ATOM	2712		HIS	363	33.898	67.568	25. 398	1.00 16.56	A	C
ATOM	2713		HIS	363	34. 638	67.880	26.489	1.00 16.19	. A	C
ATOM ATOM	2714		HIS	363	34. 292	66.303	25. 019	1.00 14.56	A	N
ATOM	2715 2716		HIS HIS	363 363	35. 227 35. 457	65.869	25.843	1.00 14.60 1.00 16.65	A	C
ATOM	2717	C	HIS	363	32. 364	66. 808 70. 081	26. 744 22. 903	1.00 10.03	A A	N C
ATOM	2718	Ö	HIS	363	31.535	70.709	23. 564	1.00 20.84	A	0
ATOM	2719	N	PHE	364	32. 383	70.075	21. 573	1.00 20.84	A	N
ATOM	2720	CA	PHE	364	31.416	70.832	20. 786	1.00 18.84	A	Č
ATOM	2721	CB	PHE	364	32.042	71.310	19.470	1.00 18.67	A	č
ATOM	2722	CG	PHE	364	33.073	72. 390	19.629	1.00 18.84	A	č
ATOM	2723		PHE	364	34.341	72.096	20.117	1.00 17.51	Ā	Č
ATOM	2724		PHE	364	32.776	73.708	19. 274	1.00 16.76	Ā	Ċ
ATOM	2725		PHE	364	35. 298	73. 095	20. 246	1.00 16.92	Α	C
ATOM	2726		PHE	364	33.727	74.711	19.401	1.00 16.24	Α	C
ATOM	2727		PHE	364	34.988	74. 404	19.886	1.00 16.59	Α	C
ATOM	2728	C	PHE	364	30. 172		20. 432	1.00 19.35	Α	C
ATOM	2729	0	PHE	364	30. 226	68. 831	20. 262	1.00 20.71	Α	0
ATOM	2730	N	THR	365	29.050	70. 750	20. 313	1.00 18.81	A	N
ATOM	2731	CA	THR	365	27. 805	70.113	19.912	1.00 18.11	A	Č
ATOM	2732	CB	THR	365	26.600	71.017	20. 161	1.00 17.38	A	C
ATOM	2733	0G1		365	26. 521	71.991	19.119	1.00 22.40	A	0
ATOM	2734	CG2		365	26. 741	71.734	21.487	1.00 13.72	A	C
ATOM	2735	C	THR	365	28. 001	69.954	18. 409	1.00 17.58	A	C
ATOM ATOM	$\frac{2736}{2737}$	O N	THR LEU	365 366	28. 823 27. 250	70.650 69.058	17. 824 17. 784	1.00 16.70 1.00 19.74	A	0 N
ATOM	2738	CA	LEU	366	27. 388	68. 799	16. 350	1.00 19.74	A A	N C
ATOM	2739	CB	LEU	366	26. 237	67. 923	15. 860	1.00 19.89	A	C
ATOM	2740		LEU	366	26. 338	67. 381	14. 431	1.00 19.43	A	C
ATOM	2741		LEU	366	27. 606	66. 542	14. 282	1.00 20.45	A	Ç ·
ATOM	2742		LEU	366	25. 112	66. 539	14. 128	1.00 20.40	A	Č
ATOM	2743	C	LEU	366	27. 503	70.017	15. 438	1.00 21.11	A	č

•						,	
					FIG. 4-57	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2744 2745 2746 2747 2748 2749 2750 2751 2752 2753 2756 2756 2757 2768 2761 2762 2763 2764 2765 2766 2767 2768 2769 2770 2771 2772 2773 2774 2775	N CAC CB CG ODD C O N CAC CB CG OD NCAC CB CCD NCAC CB	ASP ASP ASP ASP GLYY ASS ASP GLYY ASS ASS ASS ASS ASS ASS ASS ASS ASS A	367 367 367 368 368 368 369 369 369 369 369 369 370 370 370 371 371 371 371 371	28. 269 69. 989 14. 476 1. 00 24. 21 26. 764 71. 084 15. 722 1. 00 21. 26 26. 830 72. 261 14. 867 1. 00 22. 95 25. 567 73. 114 15. 005 1. 00 26. 09 25. 458 73. 796 16. 355 1. 00 29. 82 26. 469 73. 849 17. 094 1. 00 28. 76 24. 352 74. 296 16. 669 1. 00 31. 88 28. 047 73. 130 15. 139 1. 00 22. 76 28. 274 74. 122 14. 448 1. 00 25. 46 28. 818 72. 772 16. 155 1. 00 21. 02 30. 001 73. 541 16. 480 1. 00 18. 54 29. 740 74. 946 16. 987 1. 00 17. 42 30. 678 75. 690 17. 237 1. 00 17. 82 28. 482 75. 324 17. 164 1. 00 17. 57 28. 196 76. 669 17. 647 1. 00 17. 82 26. 838 77. 129 17. 144 1. 00 18. 92 26. 797 77. 234 15. 649 1. 00 22. 41 27. 657 77. 871 15. 038 1. 00 23. 56 25. 798 76. 606 15. 038 1. 00 23. 56 25. 798 76. 606 15. 038 1. 00 23. 56 25. 798 76. 606 15. 038 1. 00 16. 27 28. 185 77. 949 19. 665 1. 00 16. 44 28. 432 75. 742 19. 882 1. 00 15. 67 28. 533 75. 824 21. 330 1. 00 16. 34 27. 145 75. 766 21. 971 1. 00 14. 45 28. 533 75. 824 21. 330 1. 00 16. 34 27. 145 75. 766 21. 971 1. 00 16. 66 29. 565 73. 701 21. 058 1. 00 18. 15 29. 910 74. 742 23. 014 1. 00 17. 09 30. 735 73. 660 23. 532 1. 00 16. 28 32. 194 73. 808 23. 062 1. 00 14. 83 32. 881 75. 062 23. 546 1. 00 11. 31 32. 799 76. 243 22. 818 1. 00 11. 07	A A A A A A A A A A A A A A A A A A A	Continued) O N C C C O O C O N C C C O N C C C O N C C C O N C C C C
ATOM ATOM ATOM ATOM ATOM	2777 2778 2779 2780 2781	CE1	PHE PHE PHE PHE PHE	371 371 371 371 371 371	33. 465 77. 409 23. 256 1. 00 12. 04 A 34. 302 76. 205 25. 178 1. 00 9. 92 A 34. 219 77. 383 24. 444 1. 00 9. 76 A 30. 703 73. 545 25. 048 1. 00 16. 26 A	() () ()	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2782 2783 2784 2785 2786 2787 2788 2789 2790	N CA CB CG CD1 CE1	TYR TYR TYR TYR TYR TYR TYR TYR	372 372 372 372 372 372 372 372 372 372	30. 362 74. 495 25. 752 1. 00 15. 15 A 31. 053 72. 360 25. 536 1. 00 16. 67 A 31. 091 72. 089 26. 962 1. 00 16. 84 A 30. 349 70. 801 27. 271 1. 00 16. 79 A 28. 892 70. 879 26. 914 1. 00 18. 47 A 28. 470 70. 744 25. 589 1. 00 16. 97 A 27. 129 70. 850 25. 255 1. 00 19. 91 A 27. 931 71. 124 27. 901 1. 00 18. 26 A 26. 592 71. 235 27. 581 1. 00 19. 23 A 26. 193 71. 097 26. 258 1. 00 21. 51 A 24. 860 71. 210 25. 944 1. 00 23. 32 A	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	
ATOM	2792	C .	TYR	372	24. 860 71. 210 25. 944 1. 00 23. 32 A 32. 547 71. 977 27. 367 1. 00 18. 35 A	C 0	

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					FΙ	G. 4	- 58			(Continued)
ATOM	2793	0	TYR		33.388	71.557	26. 571	1.00 20.30	A	0
ATOM	2794	N	LYS		32.845	72.325	28. 611	1.00 18.89	Α	N
ATOM	2795	CA	LYS		34. 224	72. 318	29.071	1.00 19.69	A	C
ATOM ATOM	2796 2797	CB CG	LYS LYS		34.907	73. 541	28. 459	1.00 19.69	A	C
ATOM	2798	CD	LYS		36. 302 36. 658	73.863	28.889	1.00 20.48	A	C
ATOM	2799	CE	LYS		38. 048	75. 193	28. 240	1.00 23.59	A	C
ATOM	2800	NZ	LYS		38. 103	75. 703 77. 196	28. 601 28. 404	1.00 25.15 1.00 24.26	A	C
ATOM	2801	C	LYS		34. 277	72.369	30. 593	1.00 24.26	A	N C
ATOM	2802	ŏ	LYS		33. 474	73. 050	31. 231	1.00 20.20	A A	C 0
ATOM	2803	Ň	ILE		35. 215	71.634	31. 176	1.00 21.08	A	N
ATOM	2804	CA	ILE		35. 358	71.624	32. 621	1.00 19.63	A	Č
ATOM	2805	CB	ILE		35.960	70.309	33. 123	1.00 19.72	A	č
ATOM	2806	CG2	! ILE		36.100	70.361	34.650	1.00 19.46	A	č
ATOM	2807	CG1	ILE		35.095	69.128	32.667	1.00 19.17	Ä	č
ATOM	2808	CD1			35.652	67.753	33.079	1.00 15.57	Ā	Č
ATOM	2809	C	ILE		36.290	72.745	33.046	1.00 19.75	Α.	C
ATOM	2810	0	ILE		37.408	72.846	32.551	1.00 21.23	Α	0
ATOM	2811	N	ILE	375	35. 824	73. 595	33. 951	1.00 20.12	Α	N
ATOM	2812	CA	ILE	375	36.643	74. 684	34. 456	1.00 20.15	Α	C
ATOM	2813	CB	ILE	375	36.396	76.014	33. 700	1.00 20.38	A	C
ATOM ATOM	2814 2815		ILE ILE		36.685	75. 837	32. 215	1.00 20.24	A	C
ATOM	2816		ILE	375 375	34. 966 34. 645	76. 488	33. 919	1.00 20.36	Α.	C C C C
ATOM	2817	C	ILE	375	36.346	77. 772 74. 893	33. 186 35. 929	1.00 21.00	A	C
ATOM	2818	ő	ILE	375	35. 283	74. 512	36. 426	1.00 21.63 1.00 21.72	A	
ATOM	2819	Ň	SER	376	37. 301	75. 481	36. 634	1.00 21.72	A A	0 N
ATOM	2820	CA	SER	376	37. 132	75. 740	38. 051	1.00 23.67	A	C
ATOM	2821	CB	SER	376	38. 449	76. 228	38. 632	1.00 21.76	A	C
ATOM	2822	0G	SER	376	38. 336	76.411	40.022	1.00 26.97	Ä	ŏ
ATOM	2823	C	SER	376	36.063	76.809	38. 210	1.00 24.46	Ä	č
ATOM	2824	0	SER	376	36.042	77. 768	37.445	1.00 27.59	A	Ö
ATOM	2825	N	ASN	377	35. 164	76.659	39. 177	1.00 25.41	Α	N
ATOM	2826	CA	ASN	377	34. 128	77. 673	39. 356	1.00 26.19	Α	C
ATOM	2827	CB	ASN	377	32. 755	77. 023	39.602	1.00 25.06	Α	C
ATOM ATOM	2828 2829	CG	ASN	377	32. 682	76. 222	40.894	1.00 22.15	A	C
ATOM	2830		ASN	377	33. 560	76. 294	41.750	1.00 23.03	A	0
ATOM	2831	C	ASN ASN	377 377	31.606	75. 457	41.039	1.00 20.01	A	N
ATOM	2832	0	ASN	377	34. 447 35. 574	78. 685 78. 733	40. 456 40. 960	1.00 28.48	A	C
ATOM	2833	N	GLU	378		79. 498	40. 822	1.00 29.51	A	0
ATOM	2834	CA	GLU	378		80. 518	41.845	1.00 30.42 1.00 33.25	A	N
ATOM	2835	CB	GLU	378		81. 390	41. 988	1.00 35.25	A A	C C
ATOM	2836	CG	GLU	378		82. 505	40. 939	1.00 30.37	A	C
ATOM	2837	CD	GLU	378		83. 430	41.148	1.00 49.20	Ä	C
ATOM	2838		GLU	378		82. 970	40.972	1.00 51.65	Ä	ŏ
ATOM	2839	0E2		378	31.312		41.489	1.00 50.97	Ä	Ŏ
ATOM	2840	C	GLU	378	34.065	79. 975	43. 208	1.00 32.75	Ä	č
ATOM	2841	0	GLU	378	34. 582	80. 718	44.040	1.00 33.80	A	0

					FΙ	G. 4	- 59			(Continued)
ATOM	2842	N	GLU	379	33.842	78. 687	43. 436	1.00 31.75	. A	N
ATOM	2843	CA	GLU	379	34. 192	78. 070	44. 709	1.00 31.73	Α	С
ATOM	2844	CB	GLU	379	33. 083	77. 141	45. 182	1.00 35.37	Α	· C
ATOM	2845	CG	GLU	379	31.752	77. 788	45.416	1.00 40.59	A	C
ATOM	2846	CD	GLU	379	30. 678	76. 751	45. 677	1.00 46.30	A	C
ATOM	2847		GLU	379	30. 363	75. 976	44. 741	1.00 48.81	Ą	0
ATOM	2848		GLU	379	30. 159	76. 700	46. 815	1.00 49.11	A	0
ATOM	2849	C	GLU	379	35. 466	77. 252	44. 589	1.00 30.70	A	C
ATOM ATOM	2850 2851	0 N	GLU GLY	379 380	35.952	76. 712	45. 578	1.00 30.56	A	0
ATOM	2852	CA	GLY	380	35.986	77. 136	43. 373	1.00 29.06	A	N C
ATOM	2853	CA	GLY	380	37. 203 36. 979	76. 377 74. 931	43. 171 42. 781	1.00 27.19 1.00 27.69	A	C C
ATOM	2854	0	GLY	380	37. 935	74. 167	42. 662	1.00 27.09	A A	0
ATOM	2855	N	TYR	381	35. 726	74. 540	42.586	1.00 26.46	A	N
ATOM	2856	CA	TYR	381	35. 434	73. 167	42. 191	1.00 26.78	A	C
ATOM	2857	CB	TYR	381	34. 175	72. 671	42. 903	1.00 26.62	A	Č
ATOM	2858	CG	TYR	381	34. 394	72. 448	44. 379	1.00 24.99	A	č
ATOM	2859		TYR	381	34.864	71. 225	44. 853	1.00 24.93	A	č
ATOM	2860		TYR	381	35. 145	71. 035	46. 204	1.00 26.71	A	č
ATOM	2861		TYR	381	34. 202	73. 486	45. 296	1.00 25.27	. A	č
ATOM	2862		TYR	381	34.480	73. 312	46.647	1.00 26.88	Ä	č
ATOM	2863	CZ	TYR	381	34.955	72.082	47.097	1.00 28.08	Ā	Č
ATOM	2864	0H	TYR	381	35. 266	71.909	48. 429	1.00 28.31	Α	0
ATOM	2865	C	TYR	381	35. 261	73.100	40.678	1.00 26.94	Α	C
ATOM	2866	0	TYR	381	34.542	73. 911	40.091	1.00 28.94	Α	0
ATOM	2867	N	ARG	382	35. 938	72.147	40.045	1.00 24.97	Α	N
ATOM	2868	CA	ARG	382	35.855	72.003	38.600	1.00 22.04	Α	C
ATOM	2869	CB	ARG	382	37.057	71. 211	38. 081	1.00 24.10	A	C
ATOM	2870	CG	ARG	382	38. 322	72.045	38. 110	1.00 24.01	A	C
ATOM	2871	CD	ARG	382	39.606	71. 237	38. 141	1.00 24.10	A	C
ATOM	2872	NE CZ	ARG	382	40.647	72.083	38. 712	1.00 23.35	A	N
ATOM ATOM	2873 2874	CZ	ARG ARG	382	41.178	73. 132	38. 096	1.00 23.31	A	Ç
ATOM	2875		ARG	382 382	40.783	73. 449	36.868	1.00 21.52	A	N
ATOM	2876	C	ARG	382	42. 052 34. 548	73. 907 71. 359	38. 738	1.00 22.46 1.00 20.92	A	N
ATOM	2877	Õ	ARG	382	34. 189	70. 270	38. 186 38. 645	1.00 20.92	A	C
ATOM	2878	N	HIS	383	33. 840	72. 068	37. 313	1.00 16.12	A A	0 N
ATOM	2879	ĊA	HIS	383	32. 545	71.647	36. 813	1.00 20.43	A	C
ATOM	2880	CB	HIS	383	31.440	72. 370	37. 581	1.00 20.33	A	C
ATOM	2881	ĊĠ	HIS	383	31.177	71. 797	38. 939	1.00 22.34	A	C
ATOM	2882		HIS	383	31.590	72. 189	40.168	1.00 21.75	A	Č
ATOM	2883	ND1		383	30. 418	70.661	39. 132	1.00 20.42	A	Ň
ATOM	2884		HIS	383	30. 374	70. 380	40. 422	1.00 22.91	A	Č
ATOM	2885	NE2		383	31.076	71. 291	41.073	1.00 22.25	Ä	Ň
ATOM	2886	C	HIS	383	32.404	71.930	35. 330	1.00 20.36	Ä	Ĉ
ATOM	2887	0	HIS	383	33. 240	72.608	34.728	1.00 19.84	Ä	Ö
ATOM	2888	N	ILE	384	31.325	71.420	34.748	1.00 19.26	A	N
ATOM	2889	CA	ILE	384	31.078	71.589	33. 329	1.00 17.93	Α	C
ATOM	2890	CB	ILE	384	30. 232	70.419	32.802	1.00 17.52	Α	C

			D. I. C					(Continued)
			FIG	i. 4	- 60			
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2891 CG2 ILE 2892 CG1 ILE 2893 CD1 ILE 2894 C ILE 2895 O ILE 2896 N CYS 2897 CA CYS 2898 C CYS 2899 O CYS 2900 CB CYS 2901 SG CYS 2901 SG CYS 2902 N TYR 2903 CA TYR 2904 CB TYR 2905 CG TYR 2906 CD1 TYR 2907 CE1 TYR 2907 CE1 TYR 2908 CD2 TYR 2909 CE2 TYR 2910 CZ TYR 2911 OH TYR 2912 C TYR	384 384 384 385 385 385 385 385 386 386 386 386 386 386 386 386	30. 928 6 30. 093 6 30. 376 7 29. 333 7 30. 950 7 30. 349 7 29. 932 7 30. 654 7 28. 760 7 28. 237 7 26. 726 7 24. 912 7 24. 912 7 24. 912 7 24. 943 7 24. 943 7 24. 943 7 24. 358 7	70. 566 69. 097 67. 865 72. 898 73. 198 73. 681 74. 953 74. 887 74. 334 76. 106 77. 640 75. 470 75. 470 75. 183 75. 183 75. 271 75. 183 76. 124 77. 640 77. 640 78. 271 79. 271 79. 271 79. 271 79. 424 79. 424 79. 424 79. 424 79. 640 79.	31. 290 33. 155 32. 909 33. 028 33. 605 32. 120 31. 745 30. 284 29. 464 31. 958 32. 569 29. 973 28. 609 28. 612 27. 228 26. 930 25. 665 24. 956 24. 686 23. 449 27. 962	1. 00 15. 28 1. 00 12. 97 1. 00 9. 57 1. 00 19. 30 1. 00 18. 50 1. 00 21. 14 1. 00 24. 26 1. 00 23. 62 1. 00 23. 61 1. 00 27. 85 1. 00 27. 85 1. 00 27. 85 1. 00 21. 88 1. 00 21. 88 1. 00 21. 89 1. 00 23. 48 1. 00 23. 55 1. 00 24. 11 1. 00 22. 70 1. 00 23. 04 1. 00 24. 39 1. 00 23. 13 1. 00 22. 02	A A A A A A A A A A A A A A A A A A A	C C C C C C C C C C C C C C C C C C C
ATOM ATOM	2912 C TYR 2913 O TYR 2914 N PHE	386	28. 187 7	6.816 7.868 6.775	27. 962 28. 493 26. 806	1.00 22.02 1.00 22.52 1.00 21.19	A A A	C O N
ATOM ATOM ATOM	2915 CA PHE 2916 CB PHE 2917 CG PHE	387 387	29. 582 7 31. 087 7	7. 988 7. 987 8. 222	26. 080 25. 781 26. 973	1.00 19.95 1.00 17.05 1.00 14.01	A A A	C C C
ATOM ATOM ATOM	2918 CD1 PHE 2919 CD2 PHE 2920 CE1 PHE	387 387	32. 547 7 32. 293 7	9. 469 7. 178 9. 672	27. 185 27. 835 28. 231	1.00 9.81 1.00 11.20 1.00 9.80	A A A	C C C C
ATOM ATOM ATOM	2921 CE2 PHE 2922 CZ PHE 2923 C PHE	387 387	33. 185 7 33. 762 7	7. 376 8. 626 8. 153	28. 885 29. 082 24. 727	1.00 10.91 1.00 9.32 1.00 20.94	A A	C
ATOM ATOM ATOM	2924 O PHE 2925 N GLN 2926 CA GLN	387 388	28. 552 7° 28. 706 7°	7. 180 9. 406	24. 055 24. 332	1.00 19.77 1.00 21.79	A A A	C O N
ATOM ATOM ATOM	2927 CB GLN 2928 CG GLN 2929 CD GLN	388 388	27. 024 80 25. 745 80	0. 343	23. 030 23. 177 22. 477	1. 00 22. 21 1. 00 23. 86 1. 00 29. 81	A A A	C C C
ATOM ATOM	2930 OE1 GLN 2931 NE2 GLN	388 388	24. 357 78 25. 356 78	8. 391 8. 913	23. 109 22. 452 24. 395	1.00 32.86 1.00 34.98 1.00 36.34	A A A	C O N
ATOM ATOM ATOM	2932 C GLN 2933 O GLN 2934 N ILE	388	29. 845 81	1.428	22. 427 22. 893 21. 415	1. 00 21. 72 1. 00 22. 74 1. 00 20. 66	A A A	C O N
ATOM ATOM ATOM	2935 CA ILE 2936 CB ILE 2937 CG2 ILE	389 389	31. 231 80 31. 466 79	0. 215 9. 617	20. 821 19. 422 19. 496	1.00 21.00 1.00 20.76 1.00 19.50	A A A	C C
ATOM ATOM	2938 CG1 ILE 2939 CD1 ILE	389	30.448 80	0.165	18. 429	1.00 19.48 1.00 19.12	A A	C C C

					FIC	G. 4	- 61			(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2940 2941 2942 2943 2944 2945 2946 2947 2950 2951 2952 2953 2954 2955 2956 2957 2958 2959	OD2 C O N CA CB CC CD CE NZ C	ILE ILE ASP ASP ASP ASP ASP LYS LYS LYS LYS LYS LYS LYS LYS	389 389 390 390 390 390 390 391 391 391 391 391 391 391 391	31. 483 32. 640 30. 423 30. 584 29. 932 28. 467 27. 754 28. 029 30. 005 29. 402 30. 163 29. 707 28. 348 27. 203 25. 867 24. 733 23. 454 30. 772 31. 192 31. 219	81. 713 82. 146 82. 505 83. 953 84. 508 84. 215 84. 955 83. 236 84. 676 85. 735 84. 078 84. 679 84. 128 84. 772 84. 772 84. 073 84. 369 83. 223 85. 401	20. 735 20. 776 20. 611 20. 533 19. 275 19. 216 18. 517 19. 858 21. 738 21. 603 22. 910 24. 150 24. 566 23. 824 24. 256 23. 413 23. 742 25. 183 25. 327 25. 888	1. 00 23. 29 1. 00 22. 48 1. 00 24. 96 1. 00 26. 49 1. 00 30. 91 1. 00 35. 45 1. 00 33. 49 1. 00 26. 43 1. 00 26. 54 1. 00 27. 05 1. 00 28. 81 1. 00 28. 62 1. 00 31. 00 1. 00 34. 06 1. 00 33. 69 1. 00 36. 51 1. 00 29. 45 1. 00 29. 66 1. 00 30. 67	A A A A A A A A A A A A A A A A A A A	C O N C C C C C C C C C N C C O N C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2960 2961 2962 2963 2964 2965 2966 2967 2968 2970 2971 2972 2973 2974 2975 2976	OD2 C O N CA	LYS LYS LYS LYS LYS LYS LYS ASP ASP ASP ASP ASP ASP CYS CYS	392 392 392 392 392 392 393 393 393 393	32. 281 33. 069 33. 516 34. 330 34. 643 35. 369 31. 824 32. 637 30. 531 30. 015 29. 052 29. 734 30. 607 29. 409 29. 309 28. 294 29. 841 29. 243	85. 248 86. 558 87. 119 86. 098 86. 588 87. 872 84. 797 84. 679 84. 548 84. 098 85. 134 86. 450 86. 475 87. 455 82. 761 82. 666 81. 731 80. 410	26. 872 26. 985 25. 636 24. 852 23. 449 23. 495 28. 248 29. 162 28. 403 29. 690 30. 271 30. 567 31. 467 29. 895 29. 546 28. 859 30. 198 30. 115	1.00 30.67 1.00 28.28 1.00 27.07 1.00 27.55 1.00 26.02 1.00 31.24 1.00 31.57 1.00 33.64 1.00 36.88 1.00 41.66 1.00 43.84 1.00 44.39 1.00 32.91 1.00 30.05 1.00 28.94	A A A A A A A A A A A A A A A A A A A	C C C C C C O O C O N C C C O O C O N C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2978 2979 2980 2981 2982 2983 2984 2985 2986 2987 2988	C O CB SG N CA CB OG1 CG2 C		394 394 394 395 395 395 395 395	28. 262 8 30. 336 7 31. 401 7 27. 570 7 26. 645 7 25. 208 7 24. 709 7 24. 289 7 27. 048 7	78. 512 79. 833 77. 779 77. 251	31. 282 32. 258 30. 033 31. 504 31. 167 32. 204 31. 647 31. 407 32. 620 32. 772 32. 036	1. 00 27. 56 1. 00 27. 11 1. 00 31. 03 1. 00 34. 42 1. 00 25. 71 1. 00 25. 01 1. 00 25. 50 1. 00 28. 36 1. 00 21. 52 1. 00 24. 22 1. 00 24. 44	A A A A A A A A A	C C S N C C C C

				FIG. 4-62	(Continued)
ATOM ATOM ATOM ATOM	2989 2990 2991 2992	CA PHE CB PHE	396 396	27. 231 77. 185 34. 084 1. 00 23. 09 A 27. 594 75. 924 34. 715 1. 00 23. 03 A 28. 138 76. 182 36. 116 1. 00 22. 19 A 29. 581 76. 617 36. 131 1. 00 23. 20 A	C C
ATOM	2993	CD1 PHE	396	30. 604 75. 697 35. 876 1. 00 22. 48 A 29. 924 77. 935 36. 415 1. 00 20. 97 A	C
ATOM	2994	CD2 PHE	396		C
ATOM ATOM ATOM	2995 2996 2997	CE1 PHE CE2 PHE CZ PHE	396	31. 949 76. 086 35. 908 1. 00 20. 26 A 31. 267 78. 331 36. 447 1. 00 21. 70 A 32. 279 77. 400 36. 194 1. 00 20. 27 A	
ATOM	2998	C PHE	396	26. 373 75. 008 34. 764 1. 00 20. 96 A	C
ATOM	2999	O PHE		25. 311 75. 412 35. 218 1. 00 20. 96 A	O
ATOM	3000	N ILE		26. 523 73. 779 34. 279 1. 00 18. 88 A	N
ATOM ATOM ATOM	3001 3002 3003	CA ILE CB ILE CG2 ILE	397 397	25. 412 72. 842 34. 262 1. 00 18. 00 A 25. 266 72. 165 32. 879 1. 00 16. 55 A	C C
ATOM ATOM ATOM	3004 3005 3006	CG1 ILE CD1 ILE C ILE		26. 366 71. 130 32. 669 1. 00 16. 02 A 26. 180 70. 327 31. 402 1. 00 17. 85 A	C C C
ATOM ATOM ATOM	3007 3008 3009	0 ILE N THR CA THR	397 398	25. 527 71. 770 35. 338 1. 00 19. 16 A 24. 787 70. 787 35. 330 1. 00 20. 44 A 26. 480 71. 956 36. 244 1. 00 18. 55 A	C O N
ATOM	3010	CB THR OG1 THR CG2 THR	398	26. 681 71. 051 37. 367 1. 00 19. 41 A	C
ATOM	3011		398	27. 624 69. 858 37. 051 1. 00 19. 56 A	C
ATOM	3012		398	28. 978 70. 321 36. 960 1. 00 22. 60 A	O
ATOM ATOM ATOM	3012 3013 3014 3015	C THR 0 THR	398 398 398	27. 221 69. 178 35. 759 1. 00 18. 50 A 27. 343 71. 899 38. 424 1. 00 20. 24 A 27. 979 72. 903 38. 104 1. 00 20. 11 A	C C O
ATOM ATOM	3016 3017	N LYS CA LYS CB LYS	399 399 399	27. 185 71. 511 39. 681 1. 00 22. 48 A 27. 795 72. 258 40. 772 1. 00 23. 72 A 27. 111 73. 618 40. 941 1. 00 24. 42 A	N C C
ATOM	3018	CG LYS	399	25. 689 73. 583 41. 462 1. 00 27. 65 A	C
ATOM	3019	CD LYS	399	25. 269 74. 996 41. 856 1. 00 30. 77 A	C
ATOM	3020	CE LYS	399	23. 861 75. 054 42. 414 1. 00 31. 89 A	C
ATOM	3021	NZ LYS	399	22. 841 74. 747 41. 377 1. 00 35. 03 A	N
ATOM	3022	C LYS	399	27. 751 71. 476 42. 077 1. 00 22. 46 A	C
ATOM	3023	O LYS	399	27. 125 70. 425 42. 154 1. 00 21. 96 A	O
ATOM	3024	N GLY	400	28. 435 71. 989 43. 093 1. 00 21. 98 A	N
ATOM	3025	CA GLY	400	28. 463 71. 319 44. 378 1. 00 22. 66 A	C
ATOM	3026	C GLY	400	29. 891 71. 115 44. 839 1. 00 24. 94 A	C
ATOM	3027	0 GLY	400	30. 831 71. 449 44. 118 1. 00 26. 10 A	O
ATOM	3028	N THR	401	30. 064 70. 566 46. 036 1. 00 25. 34 A	N
ATOM	3029	CA THR	401	31. 400 70. 335 46. 560 1. 00 26. 41 A	C
ATOM	3030	CB THR	401	31. 443 70. 541 48. 095 1. 00 27. 75 A	C
ATOM	3031	OG1 THR	401	30. 615 69. 567 48. 741 1. 00 31. 37 A	0
ATOM	3032	CG2 THR	401	30. 924 71. 927 48. 448 1. 00 27. 06 A	C
ATOM ATOM ATOM	3033 3034 3035	C THR O THR N TRP	401 401 402	31. 923 68. 945 46. 197 1. 00 24. 83 A 32. 027 68. 049 47. 036 1. 00 26. 74 A	C O N
ATOM	3036	CA TRP	402	32. 781 67. 569 44. 340 1. 00 18. 83 A 31. 741 66. 460 44. 268 1. 00 16. 39 A	C
ATOM	3037	CB TRP	402		C

			FIG. 4-63	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3039 3040 3041 3042 3043 3044 3045 3046 3047 3048 3049 3050 3051 3052 3053 3054 3055 3056 3057 3058 3059 3060 3061 3062 3063 3064 3065 3066 3067 3068 3067 3068 3069 3070 3071 3072 3073 3074 3075 3076 3077 3078 3076 3077 3078 3079 3070 3077 3078 3079 3070 3077 3078 3079 3070 3071 3072 3073 3074 3075 3076 3077 3078 3078 3079 3078 3079 3080 3081 CG	GLU VAL A VAL B VAL G1 VAL G2 VAL ILE G2 VAL ILE G1 ILE G1 ILE GLY GLY GLY ILE	30. 434 66. 886 43. 709 1. 00 17. 90 30. 037 66. 865 42. 332 1. 00 19. 16 A 28. 701 67. 320 42. 278 1. 00 20. 21 30. 679 66. 505 41. 137 1. 00 18. 78 A 29. 364 67. 345 44. 409 1. 00 17. 97 A 28. 318 67. 605 43. 562 1. 00 20. 57 27. 989 67. 425 41. 078 1. 00 18. 32 A 29. 972 66. 608 39. 943 1. 00 19. 71 A 28. 637 67. 064 39. 924 1. 00 18. 98 A 33. 208 67. 983 42. 944 1. 00 18. 09 A 32. 956 69. 117 42. 540 1. 00 18. 12 A 33. 831 67. 089 42. 191 1. 00 17. 78 A 34. 284 67. 484 40. 866 1. 00 19. 48 A 35. 776 67. 805 40. 926 1. 00 20. 26 A 36. 122 68. 824 41. 983 1. 00 21. 69 A 37. 433 69. 522 41. 721 1. 00 23. 95 A 37. 506 70. 728 42. 020 1. 00 25. 27 A 38. 384 68. 880 41. 223 1. 00 24. 57 A 34. 028 66. 516 39. 716 1. 00 19. 74 A 33. 891 65. 305 39. 916 1. 00 19. 74 A 33. 891 65. 305 39. 916 1. 00 19. 74 A 33. 891 65. 305 39. 916 1. 00 19. 74 A 33. 891 65. 305 39. 916 1. 00 12. 13 A 35. 153 65. 875 36. 836 1. 00 18. 47 A 32. 974 66. 210 34. 914 1. 00 11. 14 A 31. 683 67. 515 36. 595 1. 00 12. 13 A 35. 153 65. 875 36. 836 1. 00 18. 83 A 36. 707 64. 088 36. 323 1. 00 24. 51 A 36. 868 62. 593 36. 653 1. 00 21. 78 A 36. 868 62. 593 36. 653 1. 00 12. 13 A 36. 868 62. 593 36. 653 1. 00 12. 13 A 36. 868 62. 593 36. 653 1. 00 12. 13 A 36. 868 62. 593 36. 653 1. 00 12. 13 A 36. 868 62. 593 36. 653 1. 00 12. 13 A 36. 868 62. 593 36. 653 1. 00 12. 13 A 36. 868 62. 593 36. 653 1. 00 12. 13 A 36. 868 62. 593 36. 653 1. 00 20. 05 A 36. 868 62. 593 36. 653 1. 00 20. 05 A 36. 868 62. 593 36. 653 1. 00 12. 13 A 37. 438 63. 218 39. 079 1. 00 26. 24 A 38. 804 68. 809 34. 817 1. 00 19. 40 A 38. 804 68. 809 34. 817 1. 00 19. 40 A 38. 804 68. 809 34. 064 1. 00 19. 40 A 39. 804 68. 809 34. 064 1. 00 19. 40 A 39. 804 68. 809 34. 064 1. 00 19. 40 A 39. 806 66. 67. 805 38. 31. 81 1. 00 16. 78 A 30. 679 63. 268 32. 330 1. 00 17. 49 A 30. 30. 64. 569 29. 852 1. 00 16. 85 A 30. 679 63. 268 32. 330 1. 00 17. 49 A 31. 801 63. 392 28. 934 1. 00 18. 89 A 32. 766 62. 367 28. 945 1. 00 20. 84 A 33. 000 61. 176 28. 122 1. 00 20. 84 A 33. 000 61. 176 2	CCCCCNCCCONCCCCOOCONCCCCCONCCCCONCCCONCCCCONC

					FΙ	G. 4	- 64			(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3087 3088 3089 3090 3091 3092 3093 3094 3095 3096 3099 3100 3101 3102 3103 3104 3105 3106 3107 3110 3111 3112 3113 3114 3115 3116 3117 3118 3119 3120 3121 3122 3123 3124	CD2 C O N CA CB OG1 CG2 C O N CA CB OG CO O N CA CB OG CB CC CB CC CB CC CB CC CB CC CB CC CB CC CB CC CB CC CB CC CB CC CB CC CB CB	GLU GLU GLU ALA ALA ALA ALA LEU LEU LEU LEU LEU THR THR	408 408 408 408 409 409 409 409 410 410 410 410 411 411 411 411 411 411	32. 691 33. 457 34. 963 35. 519 35. 594 32. 262 32. 743 31. 100 30. 356 29. 797 29. 235 28. 651 28. 937 27. 634 26. 959 28. 434 26. 998 27. 453 25. 701 24. 741 23. 902 23. 017 24. 797 23. 846 23. 971 22. 952 22. 061 21. 206 20. 474 21. 158 20. 598 21. 015 21. 015 21. 015 21. 015 21. 015 21. 015 21. 015 21. 015 21. 015	59. 922 59. 860 59. 947 59. 081 60. 877 61. 097 60. 455 61. 729 61. 685 60. 294 62. 708 63. 041 63. 201 64. 207 65. 571 66. 778 67. 089 67. 987 63. 849 63. 849 63. 846 63. 561 62. 339 62. 649 61. 177 64. 787 65. 684 64. 836 65. 972 65. 827 64. 618 66. 118 67. 185 66. 118 67. 185 66. 118 67. 185 66. 118 67. 185 66. 104 64. 047 64. 243	28. 944 30. 254 30. 048 29. 337 30. 596 26. 780 25. 846 26. 671 25. 414 25. 180 25. 386 26. 413 24. 195 24. 038 23. 796 23. 617 24. 935 23. 134 22. 879 21. 758 23. 150 22. 100 22. 418 23. 498 22. 811 22. 050 22. 418 23. 498 22. 811 22. 050 22. 100 22. 418 23. 498 22. 811 22. 050 22. 153 22. 379 22. 153 22. 379 22. 153 22. 379 22. 934 24. 097 23. 975 22. 751	1. 00 21. 64 1. 00 23. 48 1. 00 26. 15 1. 00 28. 40 1. 00 25. 87 1. 00 22. 35 1. 00 23. 83 1. 00 22. 21 1. 00 20. 74 1. 00 21. 17 1. 00 20. 05 1. 00 19. 25 1. 00 19. 28 1. 00 19. 28 1. 00 20. 83 1. 00 20. 83 1. 00 20. 92 1. 00 20. 83 1. 00 20. 92 1. 00 20. 84 1. 00 19. 86 1. 00 20. 25 1. 00 20. 84 1. 00 15. 82 1. 00 15. 82 1. 00 15. 79 1. 00 14. 12 1. 00 20. 16 1. 00 21. 79 1. 00 20. 25 1. 00 21. 79 1. 00 20. 25 1. 00 21. 79 1. 00 22. 27 1. 00 25. 03 1. 00 21. 84 1. 00 22. 97 1. 00 25. 03 1. 00 21. 84 1. 00 22. 97 1. 00 25. 03 1. 00 21. 84 1. 00 22. 97 1. 00 25. 66 1. 00 24. 36 1. 00 30. 28 1. 00 30. 28 1. 00 32. 47	A A A A A A A A A A A A A A A A A A A	$\tt CCCOOCONCCCONCCCONCCOONCCOONCCCONCCCON$
ATOM ATOM	3125 3126	0D2 C	ASP ASP	413 413 413	17. 153 18. 474 20. 822	63. 515 65. 111 64. 918	22. 635 21. 904 25. 442	1.00 32.47 1.00 31.81 1.00 24.37	A A A	0 0 C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3127 3128 3129 3130 3131 3132 3133	O N CA CB CG CD1 CE1	ASP TYR TYR TYR TYR TYR	413 414 414 414 414 414 414	20. 306 21. 974 22. 672 22. 369 20. 925 20. 402 19. 071	65. 363 64. 259 63. 998 62. 572 62. 332 62. 822 62. 621	26. 470 25. 444 26. 694 27. 155 27. 520 28. 714	1.00 25.08 1.00 24.23 1.00 23.03 1.00 23.61 1.00 25.79 1.00 26.31	A A A A	O N C C C C
ATOM ATOM	3134 3135	CD2 CE2	TYR	414 414	20. 074 18. 740	61. 629 61. 424	29. 052 26. 666 26. 993	1.00 26.99 1.00 24.67 1.00 25.53	A A A	C C C

				FIG.	4 - 6 5			(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3145 CD 3146 C 3147 O 3148 N 3149 CA 3150 CB 3151 CG 3152 CD 3153 CE 3154 CD 3155 CE 3156 CZ 3157 OH 3158 C 3159 O 3160 N 3161 CA	TYR TYR LEU LEU LEU LEU LEU TYR	414 414 414 415 415 415 415 416 416 416 416 416 416 416 417 417	18. 246 61. 9 16. 925 61. 7 24. 180 64. 1 24. 811 64. 0 24. 741 64. 4 26. 174 64. 6 26. 502 66. 0 27. 945 66. 4 28. 184 67. 8 28. 208 65. 9 26. 518 63. 6 25. 926 63. 7 27. 449 62. 7 27. 963 60. 4 26. 698 59. 9 26. 297 60. 4 26. 698 59. 9 26. 297 60. 4 25. 137 59. 9 26. 297 60. 4 24. 374 58. 9 24. 754 58. 4 24. 374 58. 9 23. 252 58. 4 29. 167 62. 1 30. 117 62. 4 29. 238 62. 1 30. 472 62. 5	28. 188 23. 28. 531 24. 26. 639 240 25. 582 269 27. 809 28. 358 269 28. 745 28. 606 28. 745 29. 28. 606 43 30. 163 84 29. 149 63 30. 230 69 28. 909 26 28. 645 38 27. 410 71 26. 786 44 29. 245 75 28. 636 89 26. 784 78 30. 540 99 29. 822 38 31. 866 06 32. 544	1. 00 28. 30 1. 00 31. 69 1. 00 22. 81 1. 00 22. 74 1. 00 20. 51 1. 00 18. 28 1. 00 16. 58 1. 00 14. 79 1. 00 13. 01 1. 00 14. 04 1. 00 18. 57 1. 00 18. 31 1. 00 19. 11 1. 00 19. 69 1. 00 18. 66 1. 00 17. 78 1. 00 16. 67 1. 00 18. 58 1. 00 16. 35 1. 00 16. 35 1. 00 19. 22 1. 00 19. 27 1. 00 22. 92 1. 00 19. 08	A A A A A A A A A A A A A A A A A A A	C O C C C C C C C C C C C C C C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3166 CD	TYR TYR 1 TYR 1 TYR 2 TYR TYR TYR TYR TYR TYR ILE ILE ILE ILE ILE	417 417 417 417 417 417 417 417 417 418 418 418 418 418 418 419 419 419 419	30. 408 63. 9 29. 383 64. 2 29. 721 64. 2 28. 784 64. 4 28. 071 64. 6 27. 120 64. 8 27. 488 64. 8 26. 556 65. 0 30. 768 61. 6 29. 918 60. 8 31. 996 61. 7 32. 429 60. 9 33. 626 60. 0 34. 482 59. 7 34. 183 57. 7 34. 183 57. 7 32. 827 61. 9 33. 535 62. 8 32. 356 61. 6 32. 670 62. 5 31. 523 63. 52 30. 415 62. 84 32. 875 61. 7	81 32.970 82 34.049 13 35.399 76 36.391 22 33.718 85 34.710 08 36.040 46 37.020 15 33.747 53 34.207 06 35.379 19 35.015 37 36.241 29 34.378 67 33.964 09 36.453 75 36.190 71 37.664 38.764 38.996 43 39.562	1. 00 18. 38 1. 00 17. 93 1. 00 15. 25 1. 00 13. 14 1. 00 17. 72 1. 00 15. 27 1. 00 14. 25 1. 00 14. 06 1. 00 18. 77 1. 00 16. 60 1. 00 15. 54 1. 00 15. 54 1. 00 15. 48 1. 00 15. 48 1. 00 18. 54 1. 00 20. 83 1. 00 19. 59 1. 00 20. 34 1. 00 21. 79 1. 00 20. 37	A A A A A A A A A A A A A A A A A A A	C C C C C C C C C C C C C C C C C C C

					FΙ	G. 4	- 6 6			(Continued)
ATOM	3185	0	SER	419	32. 783	60. 503	39. 988	1.00 20.32	Α	0
ATOM	3186	N	ASN		33. 152	62.427	41.107	1.00 19.64	A	N
ATOM	3187	CA	ASN	420	33. 357	61.786	42.387	1.00 20.07	Α	C
ATOM	3188	CB	ASN	420	34.773	62.053	42.863	1.00 18.49	Α	С
ATOM	3189	CG	ASN	420	35.099	63.518	42.872	1.00 20.69	Α	С
ATOM	3190	0D1	ASN	420	34. 210	64.358	42.741	1.00 21.49	Α	0
ATOM	3191		ASN	420	36.376	63.844	43.034	1.00 21.39	Α	N
ATOM	3192	C	ASN		32.350	62.368	43.379	1.00 20.90	Α	C
ATOM	3193	0	ASN	420	32.677	62.610	44.535	1.00 21.17	Α	0
ATOM	3194	N	GLU	421	31.127	62.600	42.914	1.00 21.68	Α	N
ATOM	3195	CA	GLU	421	30.081	63.160	43.761	1.00 24.26	Α	C
ATOM	3196	CB	GLU	421	28.935	63.722	42.901	1.00 26.18	Α	C
ATOM	3197	CG	GLU	421	27.714	64.214	43.701	1.00 25.32	Α	C
ATOM	3198	CD	GLU	421	26.604	64.817	42.824	1.00 26.09	Α	C
ATOM	3199	0E1	GLU	421	25.563	65.237	43.373	1.00 24.11	Α	0
ATOM	3200	0E2	GLU	421	26.762	64.873	41.588	1.00 27.22	Α	0
ATOM	3201	C	GLU	421	29.512	62.133	44. 729	1.00 24.93	Α	C
ATOM	3202	0	GLU	421	29.185	62.457	45.868	1.00 27.30	Α	0
ATOM	3203	N	TYR	422	29.409	60.892	44.272	1.00 23.63	Α	N
ATOM	3204	CA	TYR	422	28.837	59.826	45.075	1.00 23.67	Α	C
ATOM	3205	CB	TYR	422	28. 942	58. 503	44.311	1.00 23.61	Α	C
ATOM	3206	CG	TYR	422	28.015	57.415	44.813	1.00 24.39	Α	C .
ATOM	3207		TYR	422	26.642	57. 637	44. 936	1.00 23.87	Α	C
ATOM	3208		TYR	422	25. 781	56.618	45.347	1.00 22.11	Α	C
ATOM	3209		TYR	422	28.505	56.147	45.120	1.00 24.53	Α	C
ATOM	3210		TYR	422	27. 654	55. 124	45.533	1.00 23.32	Α	C
ATOM	3211	CZ	TYR	422	26.300	55.367	45.641	1.00 23.52	Α	C
ATOM	3212	OH	TYR	422	25. 471	54. 349	46.031	1.00 24.33	Α	0
ATOM	3213	C	TYR	422	29. 399	59.679	46.493	1.00 23.57	Α	C
ATOM	3214	0	TYR	422	30. 599	59. 478	46.704	1.00 23.17	Α	0
ATOM	3215	N	LYS	423	28. 492	59. 784	47.461	1.00 23.07	Α	N
ATOM	3216	CA	LYS	423	28.813	59.661	48. 878	1.00 22.04	Α	C
ATOM	3217	CB	LYS	423	29. 156	58. 205	49. 205	1.00 24.22	Α	C
ATOM	3218		LYS	423	27. 967	57. 266		1.00 25.11	A	C
ATOM	3219	CD	LYS	423	28. 303	55.809	49. 276	1.00 26.55	A	C
ATOM	3220	CE	LYS	423	27.079	54. 930	49.002	1.00 28.11	A	C
ATOM	3221	NZ	LYS	423	27.302	53. 498	49. 336	1.00 27.79	A	N
ATOM	3222	C	LYS	423	29. 923	60. 583	49. 347	1.00 21.46	A	C
ATOM	3223	0	LYS	423	30. 533	60. 340	50. 385	1.00 20.97	A	0
ATOM	3224	N	GLY	424	30. 167	61.647	48. 583	1.00 21.39	A	N
ATOM	3225	CA	GLY	424	31. 201	62.608	48. 930	1.00 21.20	A	C
ATOM	3226	C	GLY	424	32.606	62.034	48. 961	1.00 21.98	A	C
ATOM	3227	0 N	GLY	424	33. 463	62. 534	49.687	1.00 22.19	A	0
ATOM	3228	N	MET	425 425	32. 848	60. 991	48. 173	1.00 22.44	A	N
ATOM	3229	CA	MET	425	34. 161	60. 350	48. 134	1.00 23.29	A	C
ATOM	3230	CB	MET	425	34.003	58. 826	48.056	1.00 24.14	A	C
ATOM	$\begin{array}{c} 3231 \\ 3232 \end{array}$	CG SD	MET	425 425	33. 548	58. 187	49.360	1.00 25.32	A	C
ATOM			MET	425 425	33.092	56. 451	49.179	1.00 29.39	A	S
ATOM	3233	CE	MET	425	34.663	55.611	49. 406	1.00 27.92	Α.	C

					F I G. 4 - 67	(Con	tinued)
ATOM	3234		MET	425	35. 042 60. 827 46. 986 1. 00 22. 06 A	С	
ATOM	3235	0	MET	425	34. 836 60. 457 45. 835 1. 00 22. 61 A	0	
ATOM	3236	N	PRO	426	36. 045 61. 661 47. 292 1. 00 21. 75 A	N	
ATOM	3237		PRO	426	36. 386 62. 215 48. 615 1. 00 21. 34 A	C	
ATOM	3238	CA	PRO	426	36. 951 62. 172 46. 262 1. 00 20. 07 A	C	
ATOM	3239	CB	PRO	426	37. 943 63. 007 47. 062 1. 00 20. 22 A	C	
ATOM ATOM	3240	CG	PRO	426	37. 138 63. 461 48. 245 1. 00 19. 61 A	C	
ATOM	3241 3242	C	PRO	426	37. 636 61. 019 45. 532 1. 00 20. 63 A	C	
ATOM	3243	O N	PRO GLY	426	37. 920 61. 107 44. 343 1. 00 23. 99 A	0	
ATOM	3243 3244	CA	GLY	427 427	37. 905 59. 936 46. 252 1. 00 19. 08 A	N	
ATOM	3245	CA	GLY	427	38. 552 58. 789 45. 646 1. 00 18. 03 A	C	
ATOM	3246	Ö	GLY	427	37. 601 57. 838 44. 941 1. 00 18. 93 A 37. 965 56. 706 44. 642 1. 00 21. 55 A	C	
ATOM	3247	N	GLY	428	0.0 0.00	0	
ATOM	3248	CA	GLY	428	05 115 55 110 15 55	N	
ATOM	3249	C	GLY	428	05 000 55 050	C	
ATOM	3250	ŏ	GLY	428		C	
ATOM	3251	Ň	ARG	429	04 040 55 450	0	
ATOM	3252	CA	ARG	429	0.4 0.00 PP PPO 10 000	N	
ATOM	3253	CB	ARG	429	05 505 55 405 00 111	C	
ATOM	3254	CG	ARG	429	35. 595 57. 167 39. 444 1. 00 19. 09 A 36. 577 58. 292 39. 108 1. 00 20. 57 A	C C	
ATOM	3255	CD	ARG	429	37. 385 58. 737 40. 302 1. 00 22. 65 A	C	
ATOM	3256	NE	ARG	429	38. 359 59. 769 39. 956 1. 00 25. 75 A	N	
ATOM	3257	CZ	ARG	429	39. 078 60. 445 40. 852 1. 00 26. 83 A	C	
ATOM	3258	NH1		429	38. 927 60. 204 42. 146 1. 00 26. 78 A	N	
ATOM	3259	NH2	ARG	429	39. 957 61. 356 40. 456 1. 00 26. 24 A	N	
ATOM	3260	C	ARG	429	33. 134 56. 889 39. 756 1. 00 15. 74 A	Č	
ATOM	3261	0	ARG	429	32. 976 55. 675 39. 857 1. 00 12. 14 A	Õ	
ATOM	3262	N	ASN	430	32. 256 57. 679 39. 146 1. 00 14. 98 A	N	
ATOM	3263	CA	ASN	430	31.027 57.136 38.586 1.00 17.41 A	Č	
ATOM	3264	CB	ASN	430	29. 901 57. 216 39. 622 1. 00 17. 29 A	č	
ATOM	3265	CG	ASN	430	29. 947 56. 081 40. 620 1. 00 18. 53 A	Č	-
ATOM	3266		ASN	430	29. 607 54. 938 40. 297 1. 00 16. 68 A	ŏ	
ATOM	3267		ASN	430	30. 381 56. 386 41. 840 1. 00 15. 65 A	N	
ATOM	3268	C	ASN	430	30. 564 57. 808 37. 297 1. 00 17. 98 A	Ĉ	
ATOM	3269	0	ASN	430	30. 849 58. 976 37. 043 1. 00 19. 64 A	0	
ATOM	3270	N	LEU	431	29. 840 57. 053 36. 485 1. 00 17. 00 A	N	
ATOM	3271	CA	LEU	431	29. 314 57. 576 35. 241 1. 00 17. 70 A	C	
ATOM	3272	CB	LEU	431	29. 122 56. 442 34. 231 1. 00 15. 35 A	С	
ATOM	3273	CG	LEU	431	28. 478 56. 867 32. 913 1. 00 15. 33 A	C	
ATOM	3274		LEU	431	29. 340 57. 917 32. 230 1. 00 13. 77 A	C	
ATOM	3275	CD2		431	28. 296 55. 645 32. 018 1. 00 17. 37 A	С	
ATOM	3276	C	LEU	431	27. 978 58. 279 35. 491 1. 00 19. 03 A	C	
ATOM	3277	0 N	LEU	431	27. 095 57. 750 36. 172 1. 00 17. 62 A	0	
ATOM	3278	N	TYR	432	27. 840 59. 475 34. 933 1. 00 20. 33 A	N	
ATOM	3279	CA	TYR	432	26. 620 60. 248 35. 083 1. 00 21. 23 A	C	
ATOM ATOM	3280	CB	TYR	432	26. 848 61. 442 36. 014 1. 00 22. 85 A	C	
ATOM	3281	CC	TYR	432	27. 068 61. 070 37. 464 1. 00 25. 34 A	C	
ATOM	3282	CD1	IYK	432	28. 320 60. 646 37. 921 1. 00 24. 87 A	C	

										(Continued)
					FΙ	G. 4	- 68			Collumaca
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3283 3284 3285 3286 3287 3288 3290 3291 3292 3293 3294 3295 3296 3297 3298 3299 3300 3301 3302 3303 3304 3305 3306 3307 3308 3310 3311 3312	CD2 CE2 CZ OH C O N CA CB CCD CC O N CA CB CCC CC	TYR TYR TYR TYR TYR TYR LYS	432	F I 28. 519 26. 019 26. 205 27. 454 27. 625 26. 102 26. 860 24. 802 24. 133 23. 290 22. 564 21. 843 20. 643 19. 801 23. 228 22. 367 23. 427 22. 591 23. 427 24. 412 22. 491 23. 171 21. 782 22. 274 20. 538 19. 666 18. 202 17. 227 15. 802 15. 446	60. 305 61. 142 60. 805 60. 388 60. 054 60. 743	39. 267 38. 384 39. 723 40. 161 41. 487 33. 737 32. 770 33. 695 32. 496 31. 876 30. 618 29. 907 30. 682 29. 817 32. 835 33. 707 32. 162 32. 417 32. 815 31. 715	1. 00 24. 97 1. 00 24. 85 1. 00 25. 31 1. 00 25. 88 1. 00 25. 59 1. 00 21. 26 1. 00 21. 07 1. 00 20. 78 1. 00 20. 98 1. 00 21. 14 1. 00 25. 64 1. 00 25. 30 1. 00 25. 25 1. 00 27. 99 1. 00 20. 46 1. 00 21. 41 1. 00 20. 15 1. 00 21. 18 1. 00 21. 18 1. 00 21. 15 1. 00 22. 39 1. 00 22. 04 1. 00 23. 38 1. 00 20. 81 1. 00 21. 15 1. 00 21. 15 1. 00 21. 15 1. 00 21. 15 1. 00 22. 04 1. 00 23. 38 1. 00 20. 81 1. 00 21. 40 1. 00 23. 73 1. 00 26. 08 1. 00 29. 99 1. 00 32. 10 1. 00 34. 41	A A A A A A A A A A A A A A A A A A A	(Continued) CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
ATOM ATOM	3313 3314	NE2 C	GLN GLN	435 435	14. 978 19. 891	66. 839 67. 450	29. 819 29. 743	1.00 34.05 1.00 22.81	A A A	N C
ATOM ATOM ATOM ATOM	3315 3316 3317 3318	O N CA CB	GLN LEU LEU LEU	435 436 436 436	19. 600 20. 401 20. 679 21. 152	68. 419 67. 564 68. 865 68. 714	30. 434 28. 524 27. 951 26. 508	1.00 22.20 1.00 23.57 1.00 24.55 1.00 21.18	A A A	O N C C
ATOM ATOM ATOM ATOM	3319 3320 3321 3322		LEU LEU LEU LEU	436 436 436 436	22. 456 22. 938 23. 510 19. 491	67. 939 68. 116 68. 437 69. 812	26. 332 24. 910 27. 317 28. 020	1.00 21.36 1.00 20.02 1.00 19.70	A A A	C C C
ATOM ATOM ATOM	3323 3324 3325	O N CA	LEU SER SER	436 437 437	19. 672 18. 280 17. 059	71.016 69.268 70.075	28. 168 27. 927 27. 977	1. 00 26. 85 1. 00 28. 66 1. 00 30. 22 1. 00 32. 38	A A A	C O N C
ATOM ATOM ATOM ATOM	3326 3327 3328 3329	CB OG C O	SER SER SER SER	437 437 437 437	15. 925 16. 241 16. 610 15. 805	69. 340 69. 151 70. 437 71. 352	27. 268 25. 901 29. 394 29. 577	1. 00 32. 98 1. 00 39. 22 1. 00 33. 81 1. 00 32. 20	A A A	C 0 C 0
ATOM ATOM	3330 3331	N CA	ASP ASP	438 438	17. 124 16. 772	69. 714 69. 955	30. 387 31. 784	1.00 35.36 1.00 36.00	A A	N C

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(Continued) FIG. 4-70 58.104 23.981 37.747 1.00 24.13 C **ATOM** 3381 CA CYS 444 C 23.758 56.712 37.157 1.00 22.91 ATOM 3382 C CYS 444 A 55.990 0 3383 22.855 37.573 1.00 21.72 A **ATOM** 0 CYS 444 24.396 58.018 39.219 1.00 25.50 C ATOM 3384 CYS 444 CB Α S 26.053 57.282 39.443 SG 1.00 30.81 ATOM 3385 CYS 444 Α 36.1751.00 22.64 N N 445 24.573 56.348 A ATOM 3386 LEU 35.513 1.00 22.51 C **ATOM** 3387 CA LEU 445 24.446 55.053 A 3388 CB LEU 445 24.799 55.211 34.035 1.00 19.29 A C **ATOM** 24.049 56.349 33.341 C 1.00 19.36 3389 CG LEU 445 A **ATOM** 31.934 C 24.588 56.552 1.00 16.01 A CD1 LEU 445 ATOM 3390 C 33.319 1.00 15.72 **ATOM** 3391 CD2 LEU 445 22.559 56.034 A C 25.308 53.940 36.118 1.00 23.32 **ATOM** 3392 C LEU 445 A ATOM 3393 0 LEU 445 25.203 52.783 35.718 1.00 24.58 A 0 26.148 54.274 37.087 1.00 23.95 N ATOM 3394 N SER 446 A 37.660 3395 SER 446 27.028 53.269 1.00 23.89 C **ATOM** CA A 37. 222 3396 28.469 53.555 1.00 21.87 C CB SER 446 ATOM Α 37.648 28.882 54.847 1.00 20.09 0 ATOM 3397 0GSER 446 A 39.175 C **ATOM** 3398 C SER 446 26.969 53.145 1.00 23.77 Α **ATOM** 3399 0 SER 446 27.361 52.119 39.720 1.00 24.69 A 0 3400 CYS 26.480 54.184 39.845 1.00 24.32 ATOM N 447 N A CA CYS 447 26.382 54.207 41.309 1.00 26.45 C **ATOM** 3401 A 25.836 52.946 41.997 1.00 25.99 C ATOM 3402 C CYS 447 A **CYS** 447 26.441 52.425 42.937 **ATOM** 3403 0 1.00 24.44 Α 0 CYS 25.518 55.396 41.763 1.00 27.33 ATOM 3404 CB447 A \mathbf{c} **ATOM** 3405 SG CYS 447 26.225 57.049 41.461 1.00 34.75 A S 52.456 41.528 N **ATOM** 3406 N GLU 448 24.696 1.00 25.90 A **ATOM** 24.056 51.317 42.167 C 3407 CA GLU 448 1.00 24.38 Α 22. 581 C CBGLU 51.637 42.334 1.00 23.47 **ATOM** 3408 448 Α CG 22.332 53.075 42.721 C **ATOM** 3409 GLU 448 1.00 24.60 A CD GLU **ATOM** 3410 448 22.848 53.416 44.108 1.00 27.44 C A **ATOM** 3411 OE1 GLU 448 22.617 54.562 44.559 1.00 29.17 0 A 52.548 44.751 1.00 28.81 3412 OE2 GLU 448 23.478 **ATOM** A 0 24. 201 3413 C 448 49.941 41.537 1.00 23.54 C **ATOM** GLU Α 23.722 48.970 42.104 1.00 22.25 0 ATOM 3414 0 GLU 448 A 49.844 40.377 ATOM 3415 N LEU 449 24.844 1.00 23.78 N A ATOM 3416 LEU 449 25.024 48.547 39.717 1.00 23.34 C CA A 25.988 C ATOM 3417 CB LEU 449 48.678 38.548 1.00 20.76 A 37.472 C CG 49.712 1.00 21.20 ATOM 3418 LEU 449 25.680 A **ATOM** 3419 CD1 LEU 449 26.872 49.807 36.543 1.00 20.05 C Α C **ATOM** 24.424 49.335 36.711 1.00 17.29 3420 CD2 LEU 449 A ATOM 3421 C LEU 449 25.551 47.456 40.654 1.00 24.61 Α C 40.549 ATOM 3422 0 LEU 449 25. 157 46.298 1.00 26.01 Α 0 ATOM 3423 N ASN 450 26.445 47.830 41.562 1.00 25.89 N A 3424 1.00 27.02 C ATOM CA ASN 450 27.040 46.889 42.512 A 27.939 45.913 41.754 1.00 27.92 C 3425 CB ASN 450 A **ATOM** C **ATOM** 3426 CG ASN 450 28.296 44.695 42.572 1.00 31.61 Α 3427 OD1 ASN 450 28.521 44.786 43.783 1.00 34.65 0 **ATOM** Α ND2 ASN 450 28.363 41.912 1.00 31.27 **ATOM** 3428 43.541 A N 3429 ASN 450 27.877 47.731 43.488 1.00 26.54 C ATOM C

				FIG. 4-71	(Continued)
ATOM ATOM	3430 3431	N PR	0 451	29. 099 47. 637 43. 523 1. 00 26. 25 27. 210 48. 558 44. 303 1. 00 27. 04 A	0 N
ATOM ATOM	3432 3433			25. 762 48. 411 44. 535 1. 00 27. 72 A	C .
ATOM	3434			27. 796 49. 465 45. 296 1. 00 27. 49 A 26. 579 49. 924 46. 103 1. 00 27. 21 A	C
ATOM	3435			05 600 40 505 45 600 4 60 60	C
ATOM	3436			25. 638 48. 765 45. 989 1. 00 25. 73 A 28. 938 48. 983 46. 187 1. 00 28. 75 A	C C
ATOM	3437			29. 877 49. 737 46. 433 1. 00 30. 69 A	0
ATOM	3438	N GL		28. 873 47. 746 46. 666 1. 00 29. 54 A	N
ATOM	3439			29. 918 47. 228 47. 545 1. 00 30. 30 A	Č
ATOM	3440			29. 453 45. 937 48. 232 1. 00 33. 99 A	Č
ATOM	3441			28. 085 46. 024 48. 890 1. 00 39. 92 A	С
ATOM ATOM	3442			27. 817 44. 848 49. 813 1. 00 45. 87 A	C
ATOM	3443 3444			28. 084 43. 693 49. 402 1. 00 47. 97 A	0
ATOM	3445			27. 336 45. 076 50. 948 1. 00 47. 68 A 31. 221 46. 946 46. 816 1. 00 29. 63 A	0
ATOM	3446				C
ATOM	3447	N AR		01 000 10 105 15 000 1 5	O N
ATOM	3448	CA AR		31. 099 46. 425 45. 600 1. 00 27. 01 A 32. 244 46. 057 44. 783 1. 00 24. 90 A	C
ATOM	3449	CB ARG	G 453	31.950 44.728 44.085 1.00 23.08 A	Č
ATOM	3450	CG AR		32.952 44.337 43.018 1.00 22.92 A	
ATOM	3451	CD ARG		32.602 42.995 42.381 1.00 20.49 A	C C
ATOM ATOM	3452	NE ARO		33. 504 42. 688 41. 278 1. 00 18. 31 A	N
ATOM	3453 3454	CZ ARO NH1 ARO		33. 439 41. 595 40. 531 1. 00 18. 93 A	C
ATOM	3455	NH2 ARC		32. 510 40. 679 40. 763 1. 00 19. 77 A 34. 302 41. 425 39. 539 1. 00 18. 87 A	N
ATOM	3456	C ARC		00 000 10 001 10 000	N
ATOM	3457	0 ARG		32. 695 47. 071 43. 738 1. 00 25. 72 A 33. 809 46. 962 43. 222 1. 00 24. 32 A	C .
ATOM	3458	N CYS	-	31. 857 48. 054 43. 420 1. 00 25. 94 A	O N
ATOM	3459	CA CYS		32. 233 49. 012 42. 385 1. 00 25. 49 A	C
ATOM	3460	C CYS		32. 038 50. 473 42. 699 1. 00 24. 24 A	Č.
ATOM	3461	0 CYS		30. 922 50. 970 42. 688 1. 00 26. 79 A	Ö
ATOM ATOM	3462 3463	CB CYS		31.503 48.664 41.096 1.00 26.13 A	С
ATOM	3464	SG CYS N GLN		32. 156 47. 128 40. 401 1. 00 30. 12 A	S
ATOM	3465	CA GLN	455 455	33. 143 51. 165 42. 942 1. 00 22. 97 A 33. 105 52. 576 43. 276 1. 00 23. 69 A	N
ATOM	3466	CB GLN	455	22 526 52 771 44 722 4 22 22	C
ATOM	3467	CG GLN	455	00 504 50 108 45 501	C
ATOM	3468	CD GLN	455	32. 564 52. 187 45. 761 1. 00 24. 96 A 33. 177 52. 065 47. 150 1. 00 29. 34 A	C C
ATOM	3469	OE1 GLN	455	33. 981 52. 907 47. 574 1. 00 30. 98 A	0
ATOM	3470	NE2 GLN	455	32. 790 51. 022 47. 872 1. 00 28. 59 A	N
ATOM	3471	C GLN	455	33. 992 53. 425 42. 360 1. 00 24. 57 A	Ċ
ATOM	3472	0 GLN	455	33. 837 54. 645 42. 294 1. 00 27. 40 A	Ŏ
ATOM ATOM	3473 3474	N TYR CA TYR	456	34. 919 52. 787 41. 654 1. 00 22. 57 A	N
ATOM	3475	CA TYR CB TYR	456 456	35. 821 53. 510 40. 763 1. 00 21. 75 A	C
ATOM	3476	CG TYR	456 456	37. 270 53. 187 41. 124 1. 00 20. 47 A 38. 267 54. 282 40. 817 1. 00 21. 27 A	C
ATOM	3477	CD1 TYR	456		C
ATOM	3478	CE1 TYR	456	38. 659 55. 193 41. 808 1. 00 20. 27 A 39. 618 56. 165 41. 548 1. 00 18. 67 A	C C
				30. 310 00. 100 41. 040 1. 00 10. 01 A	U

					F I	G. 4	- 72			(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3503 3504 3505 3506 3507 3508 3509 3510 3511	CEZOH CON CA CBCCCON CA CCBCCCON CA CCBCCON CA CCBCCCON CA CCBCCON CA CC	VAL VAL VAL SER SER	456 456 456 456 457 457 457 457 457 457 457 457 457 458 458 458 459 459 459 459 459 459 459 459 459 459	38. 858 39. 812 40. 190 41. 151 35. 536 35. 944 34. 846 34. 499 33. 001 32. 147 31. 644 30. 830 31. 819 31. 008 30. 518 29. 728 35. 232 35. 842 35. 132 35. 739 37. 083 37. 510 34. 751 34. 072 34. 665 33. 722 32. 457 32. 816 31. 397 34. 309 35. 314 33. 667 34. 083	54. 385 55. 353 56. 236 57. 183 53. 061 51. 972 53. 899 53. 540 53. 717 52. 613 52. 674 51. 668 51. 512 50. 582 49. 568 54. 240 55. 293 53. 664 52. 652 54. 405 54. 949 56. 392 54. 475 54. 161 54. 835 53. 472 53. 456	39. 552 39. 284 40. 283 40. 023 39. 335 38. 931 38. 567 37. 196 36. 956 37. 512 38. 811 36. 727 37. 219 38. 507 38. 985 36. 066 36. 227 34. 901 33. 683 33. 474 32. 141 32. 621 32. 804 31. 520 30. 468 30. 568 30. 308 29. 595 29. 059 28. 831 28. 122 26. 728	1. 00 19. 29 1. 00 16. 18 1. 00 18. 92 1. 00 19. 64 1. 00 21. 96 1. 00 22. 39 1. 00 20. 82 1. 00 17. 91 1. 00 15. 58 1. 00 13. 21 1. 00 15. 62 1. 00 15. 62 1. 00 21. 27 1. 00 23. 18 1. 00 21. 74 1. 00 23. 18 1. 00 21. 74 1. 00 23. 93 1. 00 29. 63 1. 00 21. 73 1. 00 20. 08 1. 00 20. 58 1. 00 19. 99 1. 00 19. 45 1. 00 19. 99 1. 00 19. 99 1. 00 19. 99 1. 00 19. 10 1. 00 20. 30 1. 00 19. 99 1. 00 19. 13 1. 00 18. 73 1. 00 16. 25	A A A A A A A A A A A A A A A A A A A	(Continued) C C C C C C C C C C C C C C C C C C
ATOM ATOM ATOM ATOM ATOM	3512 3513 3514	CA CB OG C	SER SER SER SER SER	460 460 460 460 460	34. 970 35. 476 32. 809	52. 230 52. 194 53. 377	26. 476 25. 151 25. 883	1.00 16.33 1.00 15.85 1.00 15.70	A A A	C 0 C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3516 3517 3518 3519 3520 3521 3522 3523 3524 3525 3526	N CA CB CG CD1 CD2 CE1	PHE PHE PHE PHE PHE SER	460 461 461 461 461 461 461 461 461 462	30. 001 30. 779 28. 617 30. 190 28. 021 28. 811 31. 551 32. 686	52. 342 54. 475 54. 512 55. 921 56. 351 56. 764 56. 340 57. 158 56. 733 57. 142 54. 102 54. 234 53. 612	25. 841 25. 226 24. 398 24. 367 25. 660 26. 735 25. 804 27. 931 26. 996 28. 061 22. 971 22. 514 22. 269	1. 00 14. 81 1. 00 16. 00 1. 00 16. 27 1. 00 15. 50 1. 00 15. 11 1. 00 14. 16 1. 00 12. 94 1. 00 12. 76 1. 00 11. 01 1. 00 17. 94 1. 00 17. 07 1. 00 19. 22	A A A A A A A A A	O N C C C C C C C C C N

					F I G. 4 - 73	(Contin	ued)
ATOM ATOM	3528 3529	CA CB	SER SER	462 462	30. 694 53. 212 20. 877 1. 00 23. 70 A 29. 494 52. 381 20. 399 1. 00 23. 50 A	C	
ATOM	3530	0G	SER	462	28. 308 53. 145 20. 397 1. 00 24. 06 A	Ö	
ATOM	3531	C	SER	462	30. 804 54. 496 20. 058 1. 00 24. 95 A	č	
ATOM	3532	0	SER	462	30. 572 55. 581 20. 577 1. 00 25. 95 A	Ŏ	
ATOM	3533	N	LYS	463	31. 153 54. 373 18. 784 1. 00 27. 50 A	N	
ATOM	3534	CA	LYS	463	31. 323 55. 536 17. 920 1. 00 31. 80 A	С	
ATOM	3535	CB	LYS	463	31. 587 55. 084 16. 484 1. 00 33. 43 A	C	
ATOM	3536	CG	LYS	463	33. 047 55. 199 16. 075 1. 00 35. 54 A	C	
ATOM	3537	CD	LYS	463	33. 972 54. 435 17. 007 1. 00 36. 78 A	C	
ATOM ATOM	3538 3539	CE	LYS	463	35. 433 54. 724 16. 673 1. 00 39. 20 A	C	
ATOM	3540	NZ C	LYS LYS	463 463	36. 384 54. 098 17. 641 1. 00 40. 26 A	N	
ATOM	3541	Õ	LYS	463	30. 226 56. 602 17. 934 1. 00 33. 39 A 30. 484 57. 745 17. 561 1. 00 36. 36 A	C	
ATOM	3542	N	GLU	464	00 04 5 50 054 15 55	0 N	
ATOM	3543	CA	GLU	464	29. 015 56. 254 18. 354 1. 00 33. 23 A 27. 945 57. 247 18. 410 1. 00 34. 54 A	N C	
ATOM	3544	CB	GLU	464	26. 960 57. 058 17. 256 1. 00 39. 82 A	Č	
ATOM	3545	CG	GLU	464	27. 528 57. 366 15. 882 1. 00 44. 96 A	Č	
ATOM	3546	CD	GLU	464	26. 578 56. 961 14. 772 1. 00 48. 72 A	č	
ATOM	3547		GLU	464	25. 439 57. 480 14. 752 1. 00 50. 39 A	Ŏ	
ATOM	3548		GLU	464	26. 967 56. 120 13. 926 1. 00 50. 59 A	0	
ATOM	3549	C	GLU	464	27. 186 57. 202 19. 729 1. 00 32. 77 A	C	
ATOM	3550	0	GLU	464	26. 047 57. 659 19. 814 1. 00 32. 03 A	0	
ATOM	3551	N	ALA	465	27. 823 56. 636 20. 748 1. 00 31. 17 A	N	
ATOM ATOM	3552 3553	CA	ALA	465	27. 241 56. 546 22. 081 1. 00 29. 63 A	Ċ	
ATOM	3554	CB C	ALA ALA	465 465	26. 889 57. 935 22. 577 1. 00 28. 36 A	C	
ATOM	3555	0	ALA	465 465	26. 015 55. 645 22. 164 1. 00 29. 47 A 25. 176 55. 824 23. 042 1. 00 28. 66 A	C	
ATOM	3556	N	LYS	466		0	
ATOM	3557	CA	LYS	466	25. 905 54. 678 21. 259 1. 00 28. 89 A 24. 763 53. 772 21. 274 1. 00 28. 97 A	N C	
ATOM	3558	CB	LYS	466	24. 585 53. 122 19. 899 1. 00 30. 98 A	Č	
ATOM	3559	CG	LYS	466	23. 208 52. 509 19. 649 1. 00 31. 77 A	Č	
ATOM	3560	CD	LYS	466	23. 045 52. 179 18. 171 1. 00 34. 52 A	č	
ATOM	3561	CE	ĹYS	466	21.632 51.757 17.814 1.00 35.82 A	č	
ATOM	3562	NZ		466	21. 273 50. 441 18. 404 1. 00 38. 42 A	Ň	
ATOM	3563	C	LYS	466	24. 987 52. 704 22. 339 1. 00 28. 20 A	C	
ATOM	3564	0	LYS	466	24. 040 52. 126 22. 869 1. 00 27. 93 A	0	
ATOM	3565	N	TYR	467	26. 252 52. 446 22. 646 1. 00 26. 93 A	N	
ATOM	3566	CA	TYR	467	26. 599 51. 458 23. 654 1. 00 26. 21 A	C	
ATOM ATOM	3567	CB	TYR	467	26. 955 50. 119 23. 003 1. 00 27. 94 A	C	
ATOM	3568 3569	CG CD1	TYR	467	25. 823 49. 502 22. 207 1. 00 30. 39 A	C	
ATOM	3570	CE1		467 467	25. 550 49. 917 20. 903 1. 00 29. 93 A 24. 494 49. 373 20. 184 1. 00 31. 13 A	C	
ATOM	3571	CD2		467	0.000.000.000.000.000.000.000.000.000.000	C	
ATOM	3572	CE2		467	25. 009 48. 522 22. 768 1. 00 29. 73 A 23. 953 47. 975 22. 060 1. 00 30. 29 A	C C	
ATOM	3573	CZ	TYR	467	23. 698 48. 405 20. 770 1. 00 30. 25 A	C	
ATOM	3574	0H	TYR	467	22. 625 47. 890 20. 079 1. 00 32. 01 A	0	
ATOM	3575	C	TYR	467	27. 777 51. 949 24. 470 1. 00 24. 00 A	Č	
ATOM	3576	0	TYR	467	28. 491 52. 852 24. 064 1. 00 24. 63 A	ŏ	

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				FIG. 4-74	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM	3577 3578 3579 3580 3581 3582 3583	N TYR CA TYR CB TYR CG TYR CD1 TYR CE1 TYR CD2 TYR	468 468 468 468 468 468	27. 969 51. 370 25. 641 1. 00 23. 06 A 29. 091 51. 765 26. 462 1. 00 22. 80 A 28. 801 53. 043 27. 249 1. 00 23. 88 A 27. 588 53. 011 28. 155 1. 00 24. 49 A 26. 308 53. 214 27. 646 1. 00 23. 81 A 25. 206 53. 308 28. 486 1. 00 25. 51 A 27. 734 52. 883 29. 537 1. 00 26. 39 A	N C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3584 3585 3586 3587 3588 3589 3590 3591	CE2 TYR CZ TYR OH TYR C TYR O TYR N GLN CA GLN CB GLN	468 468 468 468 469 469 469	26. 638 52. 971 30. 390 1. 00 25. 67 A 25. 380 53. 191 29. 857 1. 00 25. 81 A 24. 304 53. 334 30. 695 1. 00 25. 95 A 29. 501 50. 675 27. 411 1. 00 21. 32 A 28. 672 50. 059 28. 070 1. 00 22. 73 A 30. 800 50. 431 27. 449 1. 00 20. 26 A 31. 368 49. 429 28. 315 1. 00 19. 27 A 32. 643 48. 864 27. 695 1. 00 20. 12 A	C C O C O N C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3592 3593 3594 3595 3596 3597 3598 3599	CG GLN CD GLN OE1 GLN NE2 GLN C GLN O GLN N LEU CA LEU	469 469 469 469 469 469 470 470	33. 460 47. 993 28. 632 1. 00 21. 72 A 34. 891 47. 845 28. 169 1. 00 23. 85 A 35. 605 48. 837 28. 011 1. 00 25. 81 A 35. 322 46. 609 27. 948 1. 00 23. 84 A 31. 712 50. 158 29. 589 1. 00 19. 50 A 32. 331 51. 226 29. 549 1. 00 19. 63 A 31. 277 49. 611 30. 716 1. 00 19. 27 A	C C O N C O N
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3600 3601 3602 3603 3604 3605 3606	CB LEU CG LEU CD1 LEU CD2 LEU C LEU O LEU N ARG	470 470 470 470 470 470 470	30. 410 50. 136 32. 961 1. 00 20. 14 A 29. 442 51. 323 32. 929 1. 00 21. 50 A 28. 373 51. 132 33. 996 1. 00 19. 33 A 30. 200 52. 620 33. 184 1. 00 19. 44 A 32. 768 49. 380 32. 531 1. 00 20. 91 A 32. 785 48. 152 32. 409 1. 00 19. 97 A 33. 753 50. 050 33. 102 1. 00 22. 57 A	C C C C C O N
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3607 3608 3609 3610 3611 3612 3613 3614	CA ARG CB ARG CG ARG CD ARG NE ARG CZ ARG NH1 ARG NH2 ARG	471 471 471 471 471 471 471 471	34. 917 49. 344 33. 610 1. 00 25. 83 A 36. 137 49. 690 32. 748 1. 00 29. 78 A 35. 927 49. 386 31. 261 1. 00 31. 73 A 37. 091 49. 871 30. 426 1. 00 35. 14 A 36. 939 51. 261 30. 005 1. 00 35. 86 A 37. 961 52. 061 29. 723 1. 00 35. 39 A 39. 202 51. 606 29. 830 1. 00 37. 87 A 37. 747 53. 304 29. 321 1. 00 36. 33 A	C C C N C N N
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3615 3616 3617 3618 3619 3620 3621	C ARG O ARG N CYS CA CYS C CYS O CYS CB CYS	471 471 472 472 472 472 472	35. 171 49. 686 35. 064 1. 00 24. 89 A 35. 685 50. 750 35. 388 1. 00 27. 07 A 34. 794 48. 766 35. 935 1. 00 24. 59 A 34. 948 48. 925 37. 373 1. 00 25. 55 A 36. 328 48. 418 37. 806 1. 00 23. 33 A 36. 738 47. 319 37. 433 1. 00 22. 34 A 33. 812 48. 150 38. 059 1. 00 26. 66 A	C O N C C O C
ATOM ATOM ATOM ATOM	3622 3623 3624 3625	SG CYS N SER CA SER CB SER	472 473 473 473	34. 037 47. 670 39. 797 1. 00 33. 06 A 37. 049 49. 219 38. 583 1. 00 22. 51 A 38. 377 48. 809 39. 022 1. 00 23. 17 A 39. 446 49. 724 38. 414 1. 00 21. 92 A	S N C C

					FIG. 4-75		(Continued)
ATOM	3626		SER	473	39.500 50.976 39.071 1.00 23.3	9 A	0
ATOM	3627		SER	473	38. 557 48. 754 40. 536 1. 00 23. 25		·C
ATOM	3628		SER	473	39.685 48.758 41.028 1.00 24.4		0
ATOM	3629		GLY	474	37. 457 48. 697 41. 279 1. 00 23. 29	9 A	N
ATOM	3630		GLY	474	37. 573 48. 627 42. 724 1. 00 23. 9		C
ATOM	3631	C	GLY	474	36. 330 49. 075 43. 459 1. 00 24. 4	l A	C
ATOM	3632		GLY	474	35. 434 49. 658 42. 849 1. 00 25. 28	3 A	0
ATOM	3633		PRO	475	36. 257 48. 850 44. 780 1. 00 24. 58	3 A	N
ATOM	3634		PRO	475	35. 174 49. 389 45. 623 1. 00 25. 74		C
ATOM	3635	CA	PRO	475	37. 280 48. 206 45. 609 1. 00 24. 00		C
ATOM	3636	CB	PRO	475	36. 887 48. 620 47. 022 1. 00 22. 53		C
ATOM	3637	CG	PRO	475	35. 419 48. 692 46. 945 1. 00 25. 59		C
ATOM ATOM	3638	C	PRO	475	37. 397 46. 692 45. 462 1. 00 24. 86		C
ATOM	3639 3640	0 N	PRO	475	38. 294 46. 081 46. 044 1. 00 26. 60		0
ATOM	3641	N	GLY	476	36.502 46.085 44.691 1.00 24.35		N
ATOM	3642	CA C	GLY	476	36.564 44.646 44.498 1.00 23.50		C
ATOM	3643	0	GLY GLY	476	37. 324 44. 316 43. 227 1. 00 24. 87		C
ATOM	3644	N	LEU	476 477	37. 925 45. 198 42. 613 1. 00 24. 65		0
ATOM	3645	CA	LEU	477 477	37. 308 43. 054 42. 818 1. 00 24. 78		N
ATOM	3646	CB	LEU	477	38.003 42.681 41.601 1.00 25.85		C
ATOM	3647		LEU	477	37. 927 41. 171 41. 383 1. 00 26. 86 38. 661 40. 296 42. 404 1. 00 27. 45		C
ATOM	3648		LEU	477	00 000		C
ATOM	3649		LEU	477			C
ATOM	3650	C	LEU	477	0.7.000		C
ATOM	3651	ŏ	LEU	477	00.100		C
ATOM	3652	Ň	PRO	478	36. 160 43. 663 40. 405 1. 00 27. 68 38. 183 43. 792 39. 428 1. 00 27. 18		0
ATOM	3653	CD	PRO	478	39. 645 43. 637 39. 362 1. 00 27. 65		N
ATOM	3654	CA	PRO	478	37. 684 44. 505 38. 253 1. 00 25. 83	A	C
ATOM	3655	CB	PRO	478	38. 908 44. 569 37. 351 1. 00 27. 68		C
ATOM	3656	CG	PRO	478	40.023 44.676 38.335 1.00 27.43	A	C
ATOM	3657	C	PRO	478	36.509 43.806 37.591 1.00 24.68	. A . A	C
ATOM	3658	0	PRO	478	36. 464 42. 583 37. 506 1. 00 23. 74	A	C 0
ATOM	3659	N	LEU	479	35. 561 44. 600 37. 116 1. 00 24. 02	A	N N
ATOM	3660	CA	LEU	479	34. 376 44. 068 36. 465 1. 00 23. 10	A	C
ATOM	3661	CB	LEU	479	33.186 44.151 37.420 1.00 21.62	A	Č
ATOM	3662	CG	LEU	479	31.845 43.702 36.854 1.00 21.11	Ä	č
ATOM	3663		LEU	479	31.915 42.245 36.430 1.00 21.98	Ä	č
ATOM	3664		LEU	479	30.778 43.901 37.912 1.00 24.17	Ä	č
ATOM	3665	C	LEU	479	34.077 44.857 35.199 1.00 22.18	Ä	. Č
ATOM	3666	0	LEU	479	33. 942 46. 073 35. 244 1. 00 22. 27	Ä	Õ
ATOM	3667	N	TYR	480	33.978 44.160 34.073 1.00 22.51	Ä	N
ATOM	3668	CA	TYR	480	33.690 44.801 32.790 1.00 22.76	Ä	Ĉ
ATOM	3669	CB	TYR	480	34.709 44.353 31.749 1.00 22.59	Ä	č
ATOM	3670	CG	TYR	480	36. 123 44. 657 32. 147 1. 00 21. 95	Ä	č
ATOM	3671		TYR	480	36. 702 45. 885 31. 843 1. 00 22. 81	Ä	Č
ATOM	3672	CE1		480	37. 999 46. 190 32. 249 1. 00 23. 84	Ä	Č
ATOM	3673	CD2		480	36. 872 43. 733 32. 870 1. 00 22. 05	Ä	Č
ATOM	3674	CE2	TYR	480	38. 165 44. 027 33. 286 1. 00 23. 52	Ā	Č

	F	[G. 4-76		(Continued)
ATOM 3676 OH T ATOM 3677 C T ATOM 3678 O T ATOM 3678 O T ATOM 3679 N TI ATOM 3680 CA TI ATOM 3681 CB TI ATOM 3683 CG2 TI ATOM 3683 CG2 TI ATOM 3684 C TI ATOM 3685 O TI ATOM 3686 N LI ATOM 3686 N LI ATOM 3687 CA LI ATOM 3689 CG LI ATOM 3690 CD1 LI ATOM 3691 CD2 LI ATOM 3691 CD2 LI ATOM 3692 C LI ATOM 3695 CA HI ATOM 3695 CA HI ATOM 3696 CB HI ATOM 3696 CB HI ATOM 3697 CG HI ATOM 3698 CD2 HI ATOM 3700 CE1 HI ATOM 3701 NE2 HI ATOM 3701 NE2 HI ATOM 3703 O HI ATOM 3704 N SE ATOM 3705 CA SE ATOM 3706 CB SE ATOM 3707 OG SE ATOM 3708 C SE ATOM 3708 C SE ATOM 3709 O SE ATOM 3711 CA SE ATOM 3711 CA SE ATOM 3711 CA SE ATOM 3713 OG SE ATOM 3714 C SE ATOM 3715 O SE ATOM 3716 N VAI ATOM 3717 CA VAI ATOM 3718 CB VAI	YR 480 38. 723 YR 480 39. 998 YR 480 31. 968 YR 480 31. 968 HR 481 31. 473 HR 481 29. 093 HR 481 29. 196 HR 481 29. 398 HR 481 29. 746 HR 481 29. 398 HR 481 29. 746 HR 481 29. 398 HR 481 29. 482 EU 482 28. 809 EU 482 28. 316 EU 482 29. 483 EU 482 26. 981 EU 482 26. 981 EU 482 26. 610 EU 483 26. 610 EU 483 26. 610 EU 484 26. 254 EU 485 26. 003 ES 483 27. 266 ES 483	3 45. 556 33. 379 1. 0 44. 422 32. 326 1. 0 43. 239 32. 243 1. 0 45. 181 31. 577 1. 0 45. 181 31. 577 1. 0 45. 513 32. 702 1. 0 46. 905 33. 951 1. 0 46. 905 33. 951 1. 0 47. 091 30. 136 1. 0 45. 512 29. 547 1. 0 45. 922 25. 773 1. 0 45. 922 25. 773 1. 0 45. 922 25. 773 1. 0 45. 922 25. 773 1. 0 45. 922 25. 773 1. 0 46. 767 28. 643 1. 0 46. 767 28. 643 1. 0 47. 861 27. 994 1. 0 48. 459 28. 231 1. 0 48. 459 28. 231 1. 0 48. 904 31. 012 1. 0 48. 189 32. 644 1. 0 48. 382 32. 283 1. 0 49. 281 25. 987 <	00 24. 29 A 00 26. 37 A 00 23. 22 A 00 23. 50 A 00 22. 82 A 00 22. 81 A 00 23. 28 A 00 23. 28 A 00 23. 25 A 00 23. 21 A 00 23. 25 A 00 23. 21 A 00 23. 54 A 00 22. 93 A 00 23. 14 A 00 23. 20 A 00 23. 14 A 00 23. 93 A 00 22. 16 A 00 22. 49 A 00 22. 16 A 00 24. 42 A 00 25. 98 A 00 25. 15 A 00 20. 23 A 00 19. 27 A 00 20. 23 A 00 19. 27 A 00 20. 23 A 01 19. 29 A 01 19. 17 A 01 19. 29 A 02 20. 23 A 03 19. 24 A 04 A 05 20. 23 A 06 20. 23 A 07 19. 29 A 08 A 09 20. 23 A	(Continued) C O C O C O N C C C C C C C C C C C C
	L 486 18.058 L 486 18.099 L 486 16.635 L 486 17.817 L 486 16.869	52. 816 23. 380 1. 00 51. 383 23. 869 1. 00 53. 223 23. 070 1. 00 53. 655 25. 705 1. 00 54. 415 25. 887 1. 00		

			FIG. 4-77	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3725 CB ASI	N 487 N 487 N 487 N 487 N 487 N 487 N 488 488 488 488 488 488 488	17. 458 52. 464 27. 824 1. 00 20. 70 16. 587 51. 229 27. 620 1. 00 18. 89 17. 403 50. 007 27. 171 1. 00 22. 56 16. 853 48. 948 26. 864 1. 00 24. 29 18. 722 50. 158 27. 132 1. 00 20. 73 18. 354 52. 220 29. 047 1. 00 22. 59 17. 865 51. 758 30. 079 1. 00 22. 43 19. 650 52. 514 28. 929 1. 00 23. 24 20. 606 52. 290 30. 015 1. 00 23. 32 20. 415 53. 304 31. 148 1. 00 24. 08 20. 780 54. 718 30. 750 1. 00 24. 71 21. 933 54. 956 30. 345 1. 00 25. 68 19. 907 55. 601 30. 862 1. 00 26. 77 20. 488 50. 883 30. 608 1. 00 24. 38 20. 709 50. 689 31. 803 1. 00 24. 38 20. 127 49. 902 29. 791 1. 00 24. 63 20. 099 48. 541 30. 300 1. 00 25. 48 18. 837 47. 817 <	A C C A C C A O N A C C A O A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A C C A A C C A C C A C C A C C A C C A C C A C C A C C A C C A C C A C C A C C A C C A C C A C C A C C A C C A C C A C C A C C A C C A C C A C C A C C A C C A C C A C C A C C A C C A C C A C C A C C A C C A C C A C C A C C A C C A C C A C C A C C A C C A C C A C C A C C A C C A C C A C C A C C A C C A C C A C C C A C C C A C C C A C C C A C C C A C C C A C C C A C C C A C C C A C C C A C C C A C C C A C C C A C C C C C C C C C C C C C C C C C C C C
ATOM ATOM	3762 CB ARG 3763 CG ARG	492	26. 045 40. 524 28. 648 1. 00 24. 82	A C
ATOM ATOM	3764 CD ARG	492 492	27. 159 40. 919 27. 666 1. 00 26. 62 27. 105 40. 081 26. 387 1. 00 26. 76	A C
ATOM	3766 CZ ARG	492 492	25. 884 40. 357 25. 641 1. 00 29. 45 25. 708 41. 414 24. 855 1. 00 30. 52	A N A C
ATOM ATOM	3767 NH1 ARG 3768 NH2 ARG	492 492	26. 684 42. 297 24. 692 1. 00 31. 57 24. 540 41. 610 24. 261 1. 00 29. 62	A N
ATOM ATOM	3769 C ARG 3770 O ARG	492 492	27. 117 41. 831 30. 473 1. 00 23. 83	A C
ATOM	3771 N VAL	493	27. 602 42. 958 30. 438 1. 00 22. 78 27. 680 40. 807 31. 109 1. 00 24. 93	A O A N
ATOM .	3772 CA VAL	493	28. 966 40. 911 31. 791 1. 00 25. 89	A C

	٠.				FIG	. 4-7	8			(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3773 3774 3775 3776 3777 3778 3779 3780 3781 3782 3783 3784 3785 3786 3787 3791 3792 3793 3794 3795 3797	CB CG1 CG2 C O N CA CB CD1 CD2 C O N CA CB CC O O E1 OE2 C O O CA CB CC CD O CA CB CC CD O CA CB CC CC CD O CB CC CC CC CC CC CC CC CC CC CC CC CC	VAL VAL LEU LEU LEU LEU LEU LEU GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP ASP	493 493 493 493 494 494 494 494 495 495 495 495 495 495	29. 018 44 30. 401 44 27. 977 46 30. 022 46 29. 858 31 31. 103 4 32. 154 46 32. 657 47 31. 611 47 32. 017 43 33. 315 46 34. 001 31 34. 001 31 35. 969 46 37. 153 31 37. 332 38 37. 263 37 37. 263 37 37. 539 37 34. 357 46 34. 358 39 34. 093 39 32. 761 38	0. 034 33. 0. 104 33. 0. 482 34. 0. 382 30. 9. 307 30. 1. 125 30. 0. 705 29. 1. 913 28. 2. 554 28. 3. 989 27. 1. 706 26. 0. 034 30. 9. 182 29. 0. 420 31. 9. 859 32. 0. 445 32. 0. 938 32. 0. 445 32. 0. 938 32. 1. 724 33. 7. 724 33. 7. 724 33. 7. 962 31. 0. 210 33. 1. 380 34. 0. 197 34. 0. 197 34. 0. 409 36. 3. 757 36.	052 1.00 667 1.00 044 1.00 823 1.00 250 1.00 644 1.00 944 1.00 944 1.00 944 1.00 697 1.00 453 1.00 453 1.00 453 1.00 453 1.00 453 1.00 760 1.00 862 1.00 760 1.00 596 1.00 951 1.00 285 1.00 951 1.00 285 1.00 602 1.00	0 25. 39 0 25. 35 0 25. 35 0 26. 28 0 26. 28 0 25. 35 0 22. 34 0 22. 82 0 22. 34 0 24. 93 0 24. 61 0 27. 02 0 29. 02 0 29. 20 0 24. 93 0 25. 38 0 25. 38 0 27. 01 0 27. 01	A A A	C C C C C C C C C C C C C C C C C C C
ATOM ATOM ATOM	3798 3799 3800 3801 3802 3803 3804 3805	CG OD1 OD2 C O N CA CB CG OD1 ND2 C O N CA CB OG C O N CA CB C C C C C C C C C C C C C C C C C	ASP ASP ASP ASP ASN ASN ASN ASN ASN	496 496 496 496 496 497 497 497 497 497 497 498 498 498 498 498 499 499 499	32. 814 37 31. 755 36 33. 898 36 35. 213 38 35. 177 36 36. 201 38 37. 329 37 38. 047 38 39. 988 39 38. 628 40 36. 946 36 37. 407 36 36. 108 35 35. 666 34 34. 644 33 35. 666 34 37. 056 33 37. 638 33 37. 638 33 37. 638 33 38. 814 32 39. 626 32 39. 657 33	7. 236 36. 7. 236 36. 8. 611 36. 8. 657 36. 8. 889 37. 9. 071 38. 8. 234 36. 7. 717 37. 8. 863 37. 9. 622 37. 9. 093 36. 9. 672 38. 9. 669 39. 9. 669 39. 9. 721 37. 9. 629 38. 9. 721 37. 9. 629 38. 9. 721 37. 9. 629 38. 9. 721 37. 9. 629 38. 9. 721 37. 9. 629 38. 9. 721 37. 9. 629 38. 9. 721 37. 9. 629 38. 9. 721 37. 9. 629 38. 9. 721 37. 9. 629 38. 9. 721 37. 9. 629 38. 9. 721 37. 9. 721 37. 9. 722 39. 9. 723 39. 9. 724 37. 9. 725 39. 9. 726 39. 9. 727 37. 9. 727 37. 9. 728 39. 9. 728 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39. 9. 729 39.	567 1.00 759 1.00 360 1.00 127 1.00 345 1.00 528 1.00 287 1.00 998 1.00 630 1.00 630 1.00 792 1.00 301 1.00 444 1.00 869 1.00 974 1.00 974 1.00 974 1.00 974 1.00 974 1.00 974 1.00 974 1.00 974 1.00 974 1.00 974 1.00 974 1.00 974 1.00 974 1.00 974 1.00	27. 71 27. 71 30. 85 29. 23 27. 65 27. 52 27. 52 29. 40 28. 73 29. 26 27. 48 31. 42 31. 77 31. 32 32. 01 35. 01 30. 55 31. 44 29. 46 29. 46 29. 47 30. 28 30. 98	A A A A A A A A A A A A A A A A A A A	C C C C C C C C C C C C C C C C C C C

				FΙ	G. 4	- 79			(Continue	d)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3827 CD 3828 C 3829 O 3830 N 3831 CA 3832 CB 3833 CG 3834 OD 3835 OD 3836 C 3837 O 3838 N 3839 CA 3841 CG 3842 CD 3843 CE 3844 NZ 3845 C 3846 O 3847 N 3848 CA 3849 CB 3850 CG 3851 SD 3852 CE 3853 C 3854 O 3855 N 3856 CA 3857 CB 3858 CG	ASP ASP ASP LYS LYS LYS LYS LYS LYS LYS MET MET MET MET MET MET MET LEU LEU LEU LEU	500 500 500 500 500 500 501 501	40. 098 40. 919 41. 218 42. 106 43. 459 40. 251 40. 878 38. 984 38. 294 36. 815 36. 068 36. 349 35. 202 38. 432 38. 622 38. 352 38. 470 38. 206 37. 853 39. 071 38. 700 37. 783 39. 866 40. 001 40. 900 42. 280 43. 256 43. 267 44. 396 45. 957 42. 551 43. 059 42. 215 42. 412 41. 914 42. 960	34. 393 35. 073 36. 502 37. 312 36. 635 38. 711 35. 096 34. 772 35. 484 35. 522 35. 859 35. 942 36. 870 34. 149 34. 039 33. 103 31. 741 30. 746 29. 323 28. 557 27. 147 27. 155 31. 534 31. 079 31. 881 31. 735 32. 193 31. 332 32. 530 31. 990 33. 103 37. 197	39. 223 40. 208 39. 755 40. 703 40. 871 40. 155 41. 574 42. 578 41. 624 42. 905 42. 720 44. 043 44. 831 44. 300 43. 557 44. 765 42. 740 43. 237 42. 100 42. 548 43. 050 43. 516 44. 696 43. 828 44. 963 43. 528 44. 963 44. 831 44. 963 45. 790 46. 790 47. 79	1.00 30.98 1.00 31.89 1.00 31.32 1.00 31.18 1.00 29.43 1.00 33.26 1.00 33.38 1.00 35.48 1.00 40.04 1.00 42.67 1.00 44.51 1.00 44.51 1.00 44.51 1.00 44.51 1.00 44.51 1.00 44.51 1.00 47.22 1.00 47.22 1.00 47.33 1.00 47.33	A A A A A A A A A A A A A A A A A A A	(Continue N C C C C C C C C C C C C C C C C C C	d)
ATOM ATOM ATOM	3860 CD2 3861 C	LEU LEU	504 504 504	44. 111 42. 277 41. 727	36. 668 38. 376 34. 211	44. 472 44. 635 47. 199	1.00 41.70 1.00 40.64 1.00 43.78	A A A	C C C	÷
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3863 N 3864 CA 3865 CB 3866 CG 3867 CD 3868 OE1 3869 NE2		504 505 505 505 505 505 505 505	42. 056 40. 774 40. 053 38. 911 37. 767 37. 091 36. 320 37. 390	34. 664 33. 292 32. 737 31. 834 32. 574 33. 544 33. 143 34. 829	48. 298 47. 054 48. 198 47. 721 47. 059 48. 005 48. 878 47. 848	1. 00 43. 47 1. 00 44. 74 1. 00 45. 12 1. 00 47. 10 1. 00 50. 85 1. 00 52. 28 1. 00 53. 91 1. 00 53. 20	A A A A A A	O N C C C C O N	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3860 CD2 3861 C 3862 0 3863 N 3864 CA 3865 CB 3866 CG 3867 CD 3868 OE1	LEU LEU GLN GLN GLN GLN GLN GLN	504 504 505 505 505 505 505 505 505	42. 277 41. 727 42. 056 40. 774 40. 053 38. 911 37. 767 37. 091 36. 320	38. 376 34. 211 34. 664 33. 292 32. 737 31. 834 32. 574 33. 544 33. 143	44. 635 47. 199 48. 298 47. 054 48. 198 47. 721 47. 059 48. 005 48. 878	1.00 40.64 1.00 43.78 1.00 43.47 1.00 44.74 1.00 45.12 1.00 47.10 1.00 50.85 1.00 52.28 1.00 53.91	A A A A A A A	C O N C C C C	

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						a ,	0.0			(Continued)
					F 1 (G. 4	- 80			
ATOM	0071	0	CT N	EOE	40 OOG	91 069	50. 309	1.00 44.07	A	0
ATOM	3871	0 M	GLN	505	40.806	31.863			A	N N
ATOM	3872	N	ASN	506	41.970	31. 288	48. 473	1.00 43.04		
ATOM	3873	CA	ASN	506	42.907	30. 452	49. 205	1.00 43.10	A	C
ATOM	3874	CB	ASN	506	43. 301	29. 254	48. 344	1.00 47.04	A	C
ATOM	3875	CG	ASN	506	43. 962	28. 157	49. 141	1.00 50.97	A	C
ATOM	3876		ASN	506	44. 478	27. 187	48. 575	1.00 53.71	A	0
ATOM	3877		ASN	506	43. 945	28. 293	50.467	1.00 52.33	A	N
ATOM	3878	C	ASN	506	44. 156	31.211	49.635	1.00 41.53	A	C
ATOM	3879	0	ASN	506	45. 191	30.605	49.903	1.00 41.33	A	0
ATOM	3880	N	VAL	507	44.060	32. 538	49.696	1.00 39.25	A	N
ATOM	3881	CA	VAL	507	45. 186	33. 367	50.110	1.00 35.74	A	C
ATOM	3882	CB	VAL	507	45. 801	34. 155	48. 927	1.00 35.80	A	C
ATOM	3883	CG1		507	46.989	34.974	49.416	1.00 34.07	A	C
ATOM	3884		VAL	507	46. 234	33. 204	47.823	1.00 34.58	A	C
ATOM	3885	C	VAL	507	44.726	34. 369	51.154	1.00 34.07	A	C
ATOM	3886	0	VAL	507	43.617	34.887	51.080	1.00 33.19	Α	0
ATOM	3887	N	GLN	508	45.586	34.634	52.129	1.00 33.03	Α	N
ATOM	3888	CA	GLN	508	45. 272	35. 578	53. 191	1.00 31.62	Α	С
ATOM	3889	CB	GLN	508	46. 146	35.307	54. 418	1.00 31.47	Α	С
ATOM	3890	CG	GLN	508	46.034	33.894	54.970	1.00 31.59	Α	С
ATOM	3891	CD	GLN	508	46.955	33.667	56.155	1.00 30.69	Α	C
ATOM	3892		GLN	508	46.994	34.471	57.083	1.00 31.83	Α	0
ATOM	3893		GLN	508	47.696	32.568	56.130	1.00 28.80	A	N
ATOM	3894	C	GLN	508	45. 521	36.996	52.689	1.00 30.18	A	С
ATOM	3895	0	GLN	508	46. 480	37.648	53. 097	1.00 29.60	Α	0
ATOM	3896	N	MET	509	44.652	37.463	51.801	1.00 28.77	Α	N
ATOM	3897	CA	MET	509	44. 775	38. 797	51.236	1.00 28.64	Α	C
ATOM	3898	CB	MET	509	43. 744	38.993	50. 124	1.00 30.06	Α	С
ATOM	3899	CG	MET	509	44.004	38. 143	48. 896	1.00 31.71	Α	C
ATOM	3900	SD	MET	509	45. 605	38.540	48. 171	1.00 34.08	Α	S
ATOM	3901	CE	MET	509	45. 130	39.727	46. 922	1.00 30.89	A	C
ATOM	3902	C	MET	509	44.602	39.890	52. 280	1.00 27.67	Α	С
ATOM	3903	0	MET	509	43.875	39.724	53. 255	1.00 28.41	A	0
ATOM	3904	N	PR0	510		41.032		1.00 26.51	Α	N
ATOM	3905	CD	PR0	510	46. 198	41.361	50. 978	1.00 25.01	A	C
ATOM	3906	CA	PR0	510	45.180	42.150	53. 023	1.00 24.17	Α	С
ATOM	3907	CB	PRO	510	46. 401	42.985	52.672	1.00 24.51	Α	C
ATOM	3908	CG	PRO	510	46.442	42.847	51. 185	1.00 23.21	A	C
ATOM	3909	C	PRO	510	43.881	42.896	52. 741	1.00 23.17	Α	C
ATOM	3910	0	PR0	510	43. 209	42.632	51. 751	1.00 24.30	A	0
ATOM	3911	N	SER	511	43. 527	43.826	53.607	1.00 22.25	Α	N
ATOM	3912	CA	SER	511	42.315	44.592	53. 409	1.00 23.52	A	С
ATOM	3913	CB	SER	511	41.375	44. 441	54.606	1.00 21.47	A	C
ATOM	3914	0G	SER	511	42.000	44.897	55. 796	1.00 22.50	A	0
ATOM	3915	C	SER	511	42.734	46.043	53. 258	1.00 25.81	A	C
ATOM	3916	0	SER	511	43.823	46. 433	53.687	1.00 27.50	A	0
ATOM	3917	N	LYS	512	41.869	46.838	52.642	1.00 25.44	A	Ŋ
ATOM	3918	CA	LYS	512	42.148	48. 242	52. 437	1.00 24.17	Ą	C
ATOM	3919	CB	LYS	512	42. 178	48. 555	50.943	1.00 23.04	Α	С

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ATOM	3920	CG	LYS	512		50. 043	50. 621	1.00 21.12) Λ	C
ATOM	3921	CD	LYS	512		50. 249	49. 125	1.00 21.17		C C
ATOM	3922	CE	LYS	512		51.688	48. 792	1.00 21.00		C
ATOM	3923	NZ	LYS	512		51.870	47. 343	1.00 15.68		N
ATOM	3924	C	LYS	512		49. 109	53. 105	1.00 24.25		Ĉ
ATOM	3925	0	LYS	512		48. 958	52. 846	1.00 23.45		ŏ
ATOM	3926	N	LYS	513		50.017	53.960	1.00 24.50		N
ATOM	3927	CA	LYS	513		50.941	54.647	1.00 25.28		C
ATOM	3928	CB	LYS	513		51.041	56.124	1.00 26.65	5 A	C
ATOM	3929	CG	LYS	513		52.025	56.914	1.00 27.55		C
ATOM	3930	CD	LYS	513		51.577	56.954	1.00 33.11		С
ATOM	3931	CE	LYS	513		52.476	57.844	1.00 35.12		C
ATOM	3932	NZ	LYS	513		51.943	57.960	1.00 38.12		N
ATOM ATOM	3933	C	LYS	513		52.312	53. 999	1.00 26.42		C
ATOM	3934 3935	O N	LYS LEU	513 514		52. 829	53.877	1.00 28.66		0
ATOM	3936	CA	LEU	514		52.891	53.575	1.00 25.40		N
ATOM	3937	CB	LEU	514		54. 213 54. 119	52. 958 51. 536	1.00 22.53 1.00 20.88		C .
ATOM	3938	CG	LEU	514		55. 443	50. 825	1.00 20.80		C C
ATOM	3939		LEU	514		56. 242	50.662	1.00 21.02		
ATOM	3940		LEU	514		55. 153	49.476	1.00 22.59		C C
ATOM	3941	C	LEU	514		55. 151	53. 788	1.00 22.73		č
ATOM	3942	0	LEU	514		54. 981	53.844	1.00 20.65		0
ATOM	3943	N	ASP	515		56.132	54.437	1.00 23.05		N
ATOM	3944	CA	ASP	515		57.076	55. 268	1.00 25.43		C
ATOM	3945	CB	ASP	515		56. 535	56.693	1.00 27.35		C
ATOM	3946		ASP	515		57.142	57. 458	1.00 30.82		C
ATOM ATOM	3947 3948		ASP	515		56.851	58.668	1.00 32.73		0
ATOM	3949	C	ASP ASP	515 515		57. 905	56.851	1.00 32.89		0
ATOM	3950	ŏ	ASP	515		58. 462 58. 835	55. 287 54. 357	1.00 26.80 1.00 27.23		C
ATOM	3951	Ň	PHE	516		59. 230	56. 345	1.00 27.23		O N
ATOM	3952	CA	PHE	516		60. 566	56. 431	1.00 28.71	A	C
ATOM	3953	CB	PHE	516		61.590	55. 729	1.00 28.60		Č
ATOM	3954	CG	PHE	516		61.658		1.00 28.84		č
ATOM	3955	CD1	PHE	516		62.115	57. 583	1.00 29.59		Č
ATOM	3956	CD2		516	36. 297	61.242	55. 532	1.00 30.94		Ċ
ATOM	3957	CE1		516		62.157	58.116	1.00 28.99	Α	C
ATOM	3958	CE2		516		31. 279	56.058	1.00 29.88		C
ATOM	3959	CZ	PHE	516		31. 737	57. 352	1.00 29.33		С
ATOM	3960	C	PHE	516		31.024	57. 861	1.00 28.58	A	C
ATOM ATOM	3961 3962	O N	PHE	516		50. 450	58. 811	1.00 29.42	A	0
ATOM	3963	CA	ILE ILE	517 517		52. 053	57. 990	1.00 26.80	A	N
ATOM	3964	CB	ILE	517 517		32. 651 32. 410	59. 272 59. 686	1.00 28.68 1.00 27.66	A	C
ATOM	3965		ILE	517		50. 937	59. 989	1.00 27.00	A A	C C
ATOM	3966	CG1		517		32. 861	58. 581	1.00 29.30	A	C
ATOM	3967	CD1		517			58. 431	1.00 23.30	A	C
ATOM	3968	C	ILE	517		4. 132	59. 041	1.00 30.84	A	č

					FΙ	G. 4	- 82			(Continued
ATOM	3969	0	ILE	517	40. 813	64. 577	57. 898	1.00 31.70	A	0
ATOM	3970	N	ILE	518	40.616	64. 899	60. 102	1.00 32.28	A	Ŋ .
ATOM	3971	CA	ILE	518	40. 323	66. 313	59. 924	1.00 33.51	A	C
ATOM	3972	CB	ILE	518	38. 977	66. 683	60. 595	1.00 33.41	A	C
ATOM	3973		! ILE	518	38. 603	68. 125	60. 283	1.00 33.29	A	C
ATOM	3974		ILE	518	37. 871	65. 765	60.072	1.00 33.38	A	C
ATOM	3975		ILE	518	36. 535	65. 972	60. 749	1.00 33.46	A	C
ATOM	3976	C	ILE	518	41.415	67. 222	60. 455	1.00 35.00	A	C
ATOM	3977	0 N	ILE	518 510	41.883	67.069	61.580	1.00 35.82	A	0
MOTA	3978	N	LEU	519	41.824	68. 169	59. 622	1.00 36.74	A	N
ATOM ATOM	3979 3980	CA CB	LEU LEU	519	42.850	69. 126	59. 997	1.00 39.19	A	C
ATOM	3981	CG	LEU	519 519	44. 169 44. 746	68. 828 67. 413	59. 276	1.00 38.52	A	C
ATOM	3982		LEU	519	45. 996	67. 326	59. 364 58. 493	1.00 39.20	A	C
ATOM	3983		LEU	519	45.068	67.059	60. 806	1.00 39.31 1.00 39.59	A	C
ATOM	3984	CDZ	LEU	519	42. 351	70. 501	59. 591	1.00 39.39	A	C C
ATOM	3985	Õ	LEU	519	42. 102	70. 754	58. 414	1.00 40.20	A	0
ATOM	3986	N	ASN	520	42.102	71. 382	60. 574	1.00 40.93	A	N N
ATOM	3987	CA	ASN	520	41.736	72. 735	60.321	1.00 41.70	A A	C
ATOM	3988	CB	ASN	520	42.760	73. 474	59.467	1.00 42.40	A	Č
ATOM	3989	CG	ASN	520	44. 078	73. 635	60.177	1.00 46.04	A	Č
ATOM	3990		ASN	520	44. 540	72. 723	60.859	1.00 47.21	A	Ö
ATOM	3991		ASN	520	44. 697	74. 796	60.020	1.00 50.39	Ä	N
ATOM	3992	C	ASN	520	40. 384	72. 728	59.638	1.00 42.18	Ä	C
ATOM	3993	0	ASN	520	40.183	73. 388	58.620	1.00 42.15	Ä	ŏ
ATOM	3994	N	GLU	521	39.461	71.963	60. 210	1.00 41.73	Ä	Ň
ATOM	3995	CA	GLU	521	38.105	71.861	59.691	1.00 42.64	A	Ċ
ATOM	3996	CB	GLU	521	37.445	73. 245	59.660	1.00 44.72	A	č
ATOM	3997	CG	GLU	521	37.967	74. 204	60.715	1.00 48.09	Ā	Č
ATOM	3998	CD	GLU	521	38.057	73.564	62.081	1.00 50.91	A	C
ATOM	3999		GLU	521	36.994	73.245	62.661	1.00 52.95	Α	0
ATOM	4000		GLU	521	39. 194	73.374	62.568	1.00 51.94	Α	0
ATOM	4001	C	GLU	521	38. 041	71.248	58.296	1.00 40.90	Α	C
ATOM	4002	0	GLU	521	36.967	71. 171	57. 701	1.00 40.88	A	0
ATOM	4003	N	THR	522	39. 182	70.814	57.772	1.00 39.01	A	N
ATOM	4004	CA	THR	522	39. 206	70. 221	56.442	1.00 36.94	A	C.
ATOM	4005	CB	THR	522	40. 339	70.816	55. 584	1.00 38.55	Α	C
ATOM	4006	0G1		522	40. 127	72. 223	55. 431	1.00 40.51	A	0
ATOM	4007		THR	522	40. 364	70.171	54. 202	1.00 39.39	A	C
ATOM	4008	C	THR	522	39. 357	68. 706	56. 482	1.00 34.94	A	C
ATOM	4009	0 N	THR	522	40.086	68. 152	57. 305	1.00 33.48	A	0
ATOM	4010	N	LYS	523	38.653	68.045	55. 573	1.00 33.07	A	N
ATOM	4011	CA	LYS	523	38. 685	66. 597	55. 479	1.00 30.63	A	C
ATOM ATOM	4012 4013	CB CG	LYS	523	37. 357	66.105	54. 901	1.00 31.78	A	Ü
ATOM	4013	CD	LYS LYS	523 523	36.882	64.770	55.440	1.00 34.92	A	C
ATOM	4014	CE	LYS	523	35.473	64.458	54.956	1.00 37.12	A	C C C
ATOM	4016	NZ	LYS	523 523	34.473	65. 488 65. 296	55. 455 54. 972	1.00 40.20	A	
ATOM	4017	C	LYS	523	33. 111 39. 845	66. 191	54. 873 54. 576	1.00 43.74 1.00 28.84	A	N C
1110111	1011	U	מזת	040	03.040	10.191	01.010	1.00 40.04	A	U

				FIG. 4-83	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	4018 4019 4020 4021 4022 4023 4024 4025 4026 4027 4038 4031 4032 4033 4034 4035 4036 4037 4038 4040 4041 4042 4043 4044 4045 4046 4047 4048	O LYS N PHI CA PHI CB PHI CCB PHI CCD2 PHI CCC2 PHI CCC2 PHI CCC2 PHI CCC2 TRI CCA TRI	524 524 524 524 524 524 524 524 524 524	39. 962 66. 661 53. 448 1. 00 29. 90 A 40. 711 65. 329 55. 086 1. 00 26. 11 A 41. 857 64. 858 54. 334 1. 00 23. 17 A 43. 139 65. 407 54. 953 1. 00 22. 95 A 43. 394 66. 854 54. 636 1. 00 21. 14 A 43. 265 67. 830 55. 620 1. 00 18. 86 A 44. 026 68. 587 53. 040 1. 00 19. 22 A 43. 512 69. 171 55. 329 1. 00 19. 37 A 41. 872 63. 337 54. 328 1. 00 23. 15 A 42. 084 62. 703 55. 356 1. 00 22. 01 A 41. 640 62. 758 53. 156 1. 00 24. 00 A 41. 593 61. 309 53. 000 1. 00 23. 65 A 40. 875 60. 958 51. 696 1. 00 23. 74 A 39. 476 61. 452 51. 647 1. 00 24. 69 A 38. 291 60. 687 51. 893 1. 00 25. 53 A 39. 065 62. 732 51. 418 1. 00 25. 58 A 37. 195 61. 572 51. 800 1. 00 25. 58 A 37. 693 62. 815 51. 508 1. 00 25. 52 A 37. 693 62. 815 51. 508 1. 00 25. 52 A 37. 693 62. 815 51. 508 1. 00 25. 52 A 37. 693 62. 815 51. 508 1. 00 25. 52 A 37. 693 62. 815 51. 508 1. 00 25. 32 A 35. 874 61. 151 51. 990 1. 00 25. 72 A 36. 735 58. 919 52. 374 1. 00 24. 86 A 42. 927 60. 566 53. 042 1. 00 23. 39 A 43. 994 61. 127 52. 803 1. 00 24. 19 A 42. 840 59. 280 53. 347 1. 00 22. 63 A 44. 002 58. 412 53. 410 1. 00 22. 38 A 44. 715 58. 546 54. 763 1. 00 22. 15 A 43. 946 57. 946 55. 929 1. 00 24. 08 A 43. 968 56. 574 56. 178 1. 00 23. 01	
ATOM ATOM ATOM ATOM ATOM	4049 4050 4051 4052 4053	CE1 TYR CD2 TYR CE2 TYR CZ TYR OH TYR	526 526 526	43. 215 56. 017 57. 204 1. 00 25. 01 A 43. 150 58. 748 56. 747 1. 00 24. 62 A 42. 395 58. 205 57. 772 1. 00 24. 74 A 42. 426 56. 840 57. 997 1. 00 25. 67 A	C C C C
ATOM ATOM ATOM ATOM	4054 4055 4056 4057	C TYR O TYR N GLN CA GLN	526 526 527 527	41. 650 56. 303 59. 003 1. 00 25. 43 A 43. 478 56. 990 53. 251 1. 00 22. 00 A 42. 294 56. 724 53. 482 1. 00 21. 71 A 44. 353 56. 084 52. 843 1. 00 19. 68 A 43. 964 54. 697 52. 707 1. 00 20. 14 A	0 C 0 N C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	4058 4059 4060 4061 4062 4063 4064 4065	CB GLN CG GLN CD GLN 0E1 GLN NE2 GLN C GLN O GLN N MET	527 527 527 527 527 527	43. 842 54. 301 51. 238 1. 00 19. 56 A 45. 123 54. 422 50. 465 1. 00 23. 06 A 44. 986 53. 890 49. 065 1. 00 23. 49 A 44. 034 54. 222 48. 359 1. 00 25. 79 A 45. 937 53. 066 48. 648 1. 00 22. 35 A 45. 038 53. 871 53. 389 1. 00 20. 67 A 46. 172 54. 334 53. 563 1. 00 19. 72 A 44. 674 52. 659 53. 792 1. 00 21. 11 A	C C C O N C O N
ATOM	4066	CA MET	528	45. 610 51. 771 54. 460 1. 00 22. 32 A	Ċ

FIG. 4-84										(Continued)		
14OTA	4067	СЪ	MET	528	45. 372	51.753	55. 967	1.00 23.57	A	С		
ATOM	4068	CB CG	MET	528	45. 830	52. 971	56. 727	1.00 23.53	A	C		
ATOM ATOM	4068	SD	MET	528	45.605	52. 683	58. 492	1.00 23.56	A	Š		
ATOM	4009	CE	MET	528	46. 400	54. 107	59. 158	1.00 23.30	A	Č		
ATOM	4071	CE	MET	528	45. 482	50. 347	53. 974	1.00 23.25	A	č		
ATOM	4072	0	MET	528	44. 383	49. 790	53. 935	1.00 24.82	A	ŏ		
ATOM	4073	N	ILE	529	46.605	49. 751	53.600	1.00 22.51	A	Ň		
ATOM	4074	CA	ILE	529	46. 587	48. 363	53. 183	1.00 21.97	A	Ĉ		
ATOM	4075	CB	ÎLE	529	47.644	48. 078	52.116	1.00 19.54	Ä	č		
ATOM	4076			529	47. 557	46.635	51.681	1.00 18.75	A	Ċ		
ATOM	4077		ILE	529	47. 454	49.029	50. 927	1.00 21.01	A	Č		
ATOM	4078		ILE	529	46.045	49.038	50. 335	1.00 19.28	A	C		
ATOM	4079	C	ILE	529	46.937	47.620	54.465	1.00 24.02	Α	C		
ATOM	4080	Ŏ	ILE	529	48.114	47.505	54.820	1.00 25.51	Α	0		
ATOM	4081	Ň	LEU	530	45.911	47.153	55.175	1.00 24.47	Α	N		
ATOM	4082	CA	LEU	530	46.114	46.443	56.438	1.00 24.76	Α	C		
ATOM	4083	CB	LEU	530	44.915	46.640	57.370	1.00 24.08	Α	C ,		
ATOM	4084	CG	LEU	530	44.451	48.052	57.726	1.00 24.92	Α	C		
ATOM	4085	CD1	LEU	530	43.365	47.928	58.763	1.00 26.76	Α	C		
ATOM	4086	CD2	LEU	530	45.589	48.896	58. 272	1.00 25.50	Α	C		
ATOM	4087	C	LEU	530	46.337	44.953	56.241	1.00 24.39	Α	C .		
ATOM	4088	0	LEU	530	45.686	44. 319	55.411	1.00 24.58	Α	0		
ATOM	4089	N	PR0	531	47.272	44. 374	57.003	1.00 24.58	Α	N		
ATOM	4090	CD	PR0	531	48. 174	45.045	57.950	1.00 24.42	Α	C		
ATOM	4091	CA	PR0	531	47. 578	42.943	56.913	1.00 26.79	A	C		
ATOM	.4092	CB	PRO	531	48.763	42.784	57.862	1.00 26.36	Ą	C		
ATOM	4093	CG	PRO	531	48.580	43. 913	58. 838	1.00 26.79	A	C		
ATOM	4094	C	PRO	531	46. 388	42.078	57. 312	1.00 28.05	A	C		
ATOM	4095	0	PRO	531	45. 443	42. 562	57. 931	1.00 31.01	A	0		
ATOM	4096	N	PRO	532	46. 417	40. 782	56.964	1.00 28.42	A	N		
ATOM	4097	CD	PRO	532	47. 484	40.062	56. 253	1.00 28.00	A	C		
ATOM	4098	CA	PRO	532	45. 316	39.874	57. 306	1.00 28.68	A	C		
ATOM	4099	CB	PRO	532	45. 783	38. 534	56.745	1.00 28.68	A	C		
ATOM	4100	CG	PRO	532	46. 726	38. 912	55.659	1.00 28.50	A	C		
ATOM	4101	C	PRO	532	45.113	39. 799	58.814	1.00 29.80	A	C		
ATOM	4102	0 N	PRO	532	46.051	40.006 39.501	59. 579 59. 242	1.00 31.52	A ^	0 N		
ATOM ATOM	4103 4104	N CA	HIS HIS	533 533	43. 894 43. 605	39. 382	60.670	1.00 31.29 1.00 31.80	A A	N C		
ATOM	4104		HIS	533	44. 278	38. 127	61. 225	1.00 31.80	A	Č		
ATOM	4105		HIS	533	44. 270	36. 936	60. 324	1.00 29.82	A	Č		
ATOM	4100		HIS	533	45.114	36. 247	59. 641	1.00 23.23	A	C		
ATOM	4108		HIS	533	42. 966	36. 335	60.024	1.00 28.40	A	N N		
ATOM	4109		HIS	533	43. 174	35. 326	59. 197	1.00 28.67	A	Č		
ATOM	4110		HIS	533	44. 469	35. 251	58. 949	1.00 28.85	Ä	Ň		
ATOM	4111	C	HIS	533	44. 101	40.601	61.445	1.00 33.77	Ä	Č .		
ATOM	4112	ŏ	HIS	533	44. 469	40. 489	62.617	1.00 33.99	Ä	Ŏ		
ATOM	4113	Ň	PHE	534	44. 121	41.758	60. 787	1.00 35.52	A	N		
ATOM	4114		PHE	534	44. 578	42.987	61.427	1.00 37.29	A	Č		
ATOM	4115		PHE	534	44. 249	44. 203	60. 555	1.00 36.11	A	С		

					ान	G. 4	- 85			(Continued)
ATOM ATOM ATOM ATOM ATOM	4116 4117 4118 4119 4120	CD:	PHE 1 PHE 2 PHE 1 PHE 2 PHE	534 534 534 534 534	44. 510 45. 811 43. 455 46. 056	45. 523 45. 956 46. 320 47. 167 47. 530	61. 235 61. 475 61. 654 62. 124	1.00 35.46 1.00 35.65 1.00 33.35 1.00 36.55 1.00 35.26	A A A A	C C C C
ATOM ATOM ATOM ATOM ATOM ATOM	4121 4122 4123 4124 4125 4126	CZ C O N CA CB	PHE PHE PHE ASP ASP ASP	534 534 535 535 535	44. 990 43. 920 42. 705 44. 725 44. 206	47. 957 43. 158 43. 046 43. 435 43. 621 42. 541	62.541	1. 00 35. 35 1. 00 38. 07 1. 00 38. 83 1. 00 39. 27 1. 00 40. 72 1. 00 43. 14	A A A A A	C C O N C C
ATOM ATOM ATOM ATOM ATOM ATOM	4127 4128 4129 4130 4131 4132	CG OD 1	ASP ASP ASP ASP ASP LYS	535 535 535 535 535	44. 102 43. 704 43. 999 44. 614 45. 799	42. 571 43. 668 41. 499 44. 985 45. 270	67. 460 67. 912 68. 092 65. 699 65. 837	1.00 46.19 1.00 46.58 1.00 48.00 1.00 40.91 1.00 40.57	A A A A	C 0 0 C 0
ATOM ATOM ATOM ATOM ATOM	4133 4134 4135 4136 4137	CA CB CG CD CE	LYS LYS LYS LYS LYS	536 536 536 536 536 536	43. 635 43. 936 42. 675 42. 146 41. 156 40. 721	45. 822 47. 148 48. 018 48. 406 49. 566 50. 020	66. 022 66. 539 66. 572 65. 200 65. 289 63. 897	1. 00 41. 40 1. 00 42. 56 1. 00 44. 69 1. 00 47. 06 1. 00 49. 52 1. 00 50. 85	A A A A A	N C C C C
ATOM ATOM ATOM ATOM ATOM	4138 4139 4140 4141 4142 4143	NZ C O N CA CB	LYS LYS LYS SER SER SER	536 536 536 537 537	39. 965 44. 553 44. 896 44. 697 45. 277 44. 744	51. 303 47. 105 48. 147 45. 907 45. 762 44. 499	63. 921 67. 928 68. 486 68. 486 69. 820 70. 513	1.00 51.05 1.00 42.57 1.00 42.20 1.00 42.80 1.00 43.70 1.00 44.09	A A A A	N C O N C C
ATOM ATOM ATOM ATOM ATOM	4144 4145 4146 4147 4148 4149	OG C O N CA CB	SER SER SER LYS LYS LYS	537 537 537 538 538 538	45. 222 46. 796 47. 498 47. 295 48. 729 49. 024	43. 319 45. 696 46. 061 45. 230 45. 110 43. 917	69. 888 69. 737 70. 682 68. 598 68. 380 67. 470	1. 00 43. 50 1. 00 43. 27 1. 00 44. 98 1. 00 41. 93 1. 00 40. 13 1. 00 41. 29	A A A A A	0 C O N C C
ATOM ATOM ATOM ATOM ATOM ATOM	4150 4151 4152 4153 4154 4155	CG CD CE NZ C	LYS LYS LYS LYS LYS LYS	538 538 538 538 538 538	48. 521 48. 834 48. 317 46. 864 49. 280 48. 526	42. 590 41. 446 40. 140 40. 231 46. 372 47. 229	68. 013 67. 073 67. 638 67. 960 67. 741 67. 283	1. 00 42. 24 1. 00 41. 97 1. 00 42. 57 1. 00 44. 10 1. 00 38. 59 1. 00 38. 17	A A A A	C C C N C
ATOM ATOM ATOM ATOM ATOM ATOM	4156 4157 4158 4159 4160 4161	N CA CB CG CD CE	LYS LYS LYS LYS LYS LYS	539 539 539 539 539 539	50. 601 51. 263 52. 293 51. 693 50. 925 50. 209	46. 485 47. 629 48. 225 48. 838 50. 117 50. 674	67. 725 67. 116 68. 079 69. 341 69. 028 70. 258	1.00 36.92 1.00 36.43 1.00 37.32 1.00 37.42 1.00 40.01 1.00 41.64	A A A A A	N C C C C
ATOM ATOM ATOM	4162 4163 4164	NZ C O	LYS LYS LYS	539 539 539	51.121 51.943	51.014 47.110 46.137	71. 389 65. 849 65. 893	1.00 43.98 1.00 35.38 1.00 35.49	A A A	N C O

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		·	FIG. 4	8 6		(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	4165 N TYR 4166 CA TYR 4167 CB TYR 4168 CG TYR 4169 CD1 TYR 4170 CE1 TYR 4171 CD2 TYR 4172 CE2 TYR 4173 CZ TYR 4174 OH TYR 4175 C TYR 4176 O TYR 4177 N PRO 4178 CD PRO	540 51. 540 52. 540 51. 540 50. 540 49. 540 49. 540 49. 540 48. 540 47. 540 53. 540 53. 541 54. 541 54.	658 47. 747 229 47. 316 131 47. 135 204 45. 968 109 46. 078 254 45. 000 421 44. 748 576 43. 669 495 43. 800 661 42. 724 242 48. 287 130 49. 492 270 47. 772 717 46. 383	64. 719 1 63. 452 1 62. 397 1 62. 630 1 63. 488 1 63. 699 1 62. 196 1 63. 260 1 63. 260 1 62. 890 1 62. 890 1 62. 199 1 62. 199 1 62. 020 1	1.00 33.00 1.00 30.12 1.00 28.99 1.00 29.13 1.00 27.13 1.00 27.62 1.00 27.62 1.00 27.64 1.00 29.67 1.00 29.33 1.00 31.23 1.00 27.71 1.00 25.95 1.00 27.56	A N A C A C A C A C A C A C A C A C A C A C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	4179 CA PRO 4180 CB PRO 4181 CG PRO 4182 C PRO 4183 O PRO 4184 N LEU 4185 CA LEU 4186 CB LEU 4187 CG LEU 4188 CD1 LEU 4189 CD2 LEU 4190 C LEU	541 56. 541 55. 541 54. 541 53. 542 54. 542 54. 542 52. 542 51. 542 53. 542 51. 542 53. 542 54. 542 53. 542 54.	662 46.512 463 49.358 579 48.727 763 50.613 032 51.307 220 52.440 252 53.292 422 54.170 017 54.165 924 51.855	61. 148	1.00 26.81 1.00 25.92 1.00 27.83 1.00 28.03 1.00 27.70 1.00 26.55 1.00 26.11 1.00 28.68 1.00 29.38 1.00 29.52 1.00 26.16	A C A C A C A C A C A C A C A C A C A C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	4191 O LEU 4192 N LEU 4193 CA LEU 4194 CB LEU 4195 CG LEU 4196 CD1 LEU 4197 CD2 LEU 4198 C LEU 4199 O LEU 4200 N LEU 4201 CA LEU 4202 CB LEU	542 55. 543 54. 543 55. 543 56. 543 57. 543 56. 543 54. 543 54. 543 53. 544 54. 544 54. 544 54. 544 54. 544 54. 544 54.	536 51.589 263 52.097 595 50.978 080 51.474 209 52.487 537 50.303 378 53.131 283 52.819 857 54.362 098 55.436	56. 801 1 55. 651 1 54. 660 1 53. 289 1 53. 475 1 52. 441 1 54. 966 1 54. 511 1 54. 896 1 54. 278 1	1. 00 28. 00 1. 00 23. 70 1. 00 24. 11 1. 00 24. 05 1. 00 22. 45 1. 00 24. 00 1. 00 20. 16 1. 00 24. 37 1. 00 25. 72 1. 00 24. 80 1. 00 23. 74 1. 00 23. 92	A O A N A C A C A C A C A C A C A C A C A C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	4203 CG LEU 4204 CD1 LEU 4205 CD2 LEU 4206 C LEU 4207 O LEU 4208 N ASP 4209 CA ASP 4210 CB ASP 4211 CG ASP 4212 OD1 ASP 4213 OD2 ASP	544 53. 544 52. 544 54. 544 55. 545 53. 545 53. 545 52. 545 53. 545 53.	640 58.003 157 57.743 069 59.166 403 55.543 451 56.053 477 55.049 595 55.075 570 54.132 826 53.848 175 54.790	54. 581 1 54. 729 1 55. 460 1 52. 785 1 52. 400 1 51. 962 1 50. 508 1 49. 902 1 48. 444 1 47. 699 1	1. 00 22. 62 1. 00 24. 91 1. 00 24. 25 1. 00 23. 24 1. 00 23. 44 1. 00 21. 43 1. 00 20. 10 1. 00 20. 20 1. 00 20. 73 1. 00 22. 69 1. 00 19. 91	A C A C A C A C A C A C A C A C A C A C

	(Continued)			
		F	IG. 4-87	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	4215 0 ASP 4216 N VAL 4217 CA VAL 4218 CB VAL 4219 CG1 VAL 4220 CG2 VAL 4221 C VAL 4222 O VAL 4223 N TYR 4224 CA TYR	545 53. 28 545 52. 14 546 54. 26 546 54. 04 546 54. 86 546 54. 62 546 54. 49 546 54. 32 546 55. 21 547 53. 52 547 53. 70	1 56. 499 50. 078 1. 00 20. 41 9 56. 949 50. 219 1. 00 21. 14 3 57. 201 49. 524 1. 00 19. 56 3 58. 591 49. 157 1. 00 20. 20 7 59. 511 50. 090 1. 00 20. 60 6 60. 966 49. 753 1. 00 20. 01 9 59. 239 51. 533 1. 00 21. 16 0 59. 032 47. 723 1. 00 20. 28 2 58. 513 47. 048 1. 00 22. 79 4 59. 994 47. 267 1. 00 17. 64 2 60. 604 45. 957 1. 00 15. 73	A C A O A C A C A C A C A C A C A C A C
ATOM	4226 CG TYR	547 52.65 547 52.96		A C A C
ATOM ATOM		547 52.16	0 61.688 43.006 1.00 14.20	A C
ATOM	4228 CE1 TYR 4229 CD2 TYR	547 52. 513 547 54. 130	00 040 40 004	A C
ATOM	4230 CE2 TYR	547 54. 492	2 60.926 41.726 1.00 10.35	A C A C
ATOM ATOM	4231 CZ TYR 4232 OH TYR	547 53. 680 547 54. 036	61.890 41.167 1.00 12.20	A C
ATOM	4233 C TYR	547 53. 522	62.076 46.266 1.00 14.99	A 0 A C
ATOM ATOM	4234 O TYR 4235 N ALA	547 54. 49(62. 834 46. 325 1. 00 14. 47	A 0
ATOM	4236 CA ALA	548 52. 265 548 51. 879	CO OOC 40 000 4 00 10	A N
ATOM	4237 CB ALA	548 52. 493	64.109 48.247 1.00 9.78	A C A C
ATOM ATOM	4238 C ALA 4239 O ALA	548 52.163 548 52.250	64. 950 45. 923 1. 00 11. 87	A C
ATOM	4240 N GLY	548 52. 250 549 52. 308	C1 CC0 11 CCC 1 CC 12	A 0
ATOM	4241 CA GLY	549 52.556	CE 704 40 000 4 00 15 55	A N A C
ATOM ATOM	4242 C GLY	549 51.306	66. 578 43. 573 1. 00 13. 15	A Č
ATOM	4243 O GLY 4244 N PRO	549 50. 266 550 51. 365	66. 182 44. 074 1. 00 12. 86	0 <i>P</i>
ATOM	4245 CD PRO	550 51.365 550 52.533		A N
ATOM	4246 CA PRO	550 50.174	CO FOO 40 FEA 4 50 15	I C
ATOM	4247 CB PRO	550 50.693	CD 704 41 000 4 00 17 17	i C
ATOM ATOM	4248 CG PRO 4249 C PRO	550 52.145	69. 838 42. 325 1. 00 15. 06	
ATOM	4250 O PRO	550 49.074 550 49.336	67.848 42.026 1.00 15.37 A	
ATOM	4251 N CYS	551 47.849	07 040 40 500 4 00 1014	
ATOM	4252 CA CYS	551 46.684	67. 287 41. 944 1. 00 15. 67 A	
ATOM	4253 CB CYS	551 46. 424	67.796 40.525 1.00 16.53 A	
ATOM ATOM	4254 SG CYS 4255 C CYS	551 44. 792	67. 314 39. 844 1. 00 18. 29 A	. S
ATOM	4256 0 CYS	551 46. 811 551 46. 228	65. 766 41. 925 1. 00 16. 83 A	
ATOM	4257 N SER	552 47. 574	65.096 41.087 1.00 20.00 A 65.219 42.856 1.00 16.56 A	
ATOM	4258 CA SER	552 47.742	63. 785 42. 933 1. 00 16. 35 A	
ATOM	4259 CB SER	552 49.063	63. 450 43. 613 1. 00 19. 76 A	
ATOM ATOM	4260 OG SER 4261 C SER	552 49. 023 552 40. 009	63. 805 44. 987 1. 00 20. 36 A	0
ATOM		552 46. 602 552 45. 723	63. 202 43. 760 1. 00 17. 72 A 63. 929 44. 243 1. 00 17. 55 A	C 0
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					FIG.	4 - 88			(Continue	ed)
					rig.	+ 00				
ATOM	4263	N	GLN	553	46.632 61.88	35 43.926	1.00 17.07	Α	N	
ATOM	4264	CA	GLN		45.628 61.17		1.00 16.87	A	C	
ATOM	4265	CB	GLN		44.301 61.09		1.00 16.43	Ā	Ċ	
ATOM	4266	CG	GLN		43. 249 60. 29		1.00 19.53	Ā	Č	
ATOM	4267	CD	GLN		41.844 60.46		1.00 18.87	Ā	Č	
ATOM	4268	0E1			41.520 60.01		1.00 20.67	Ā	0	
ATOM	4269	NE2			40.999 61.12		1.00 18.67	Ä	Ň	
ATOM	4270	C	GLN		46.123 59.78		1.00 18.09	Ä	Ċ	
ATOM	4271	Ó	GLN		46.088 58.91		1.00 18.25	Ä	Ö	
ATOM	4272	N	LYS	554	46.589 59.56		1.00 19.53	Ä	Ň	
ATOM	4273	CA	LYS	554	47.075 58.24		1.00 20.69	Ä	Ċ	
ATOM	4274	CB	LYS	554	48.319 58.38		1.00 22.65	Ä	Č .	
ATOM	4275	CG	LYS	554	49.538 58.88		1.00 24.15	Ä	Č	
ATOM	4276	CD	LYS	554	50.064 57.84		1.00 25.21	Ä	Č	
ATOM	4277	CE	LYS	554	50.777 56.71		1.00 24.75	Ä	Č	
ATOM	4278	NZ	LYS	554	51.472 55.79		1.00 23.89	Ä	Ň	
ATOM	4279	C	LYS	554	45.996 57.47		1.00 21.48	Ä	Č	
ATOM	4280	0	LYS	554	46. 108 56. 25		1.00 22.39	Ā	Ö	
ATOM	4281	N	ALA	555	44. 952 58. 17		1.00 20.77	Ä	N	
ATOM	4282	CA	ALA	555	43.849 57.55		1.00 20.46	A	C	
ATOM	4283	CB	ALA	555	43. 525 58. 37		1.00 18.05	A	Č	
ATOM	4284	C	ALA	555	42.611 57.43		1.00 21.32	Ā	Č	
ATOM	4285	0	ALA	555	41.996 58.44		1.00 21.75	A	Ö	
ATOM	4286	N	ASP	556	42. 249 56. 20		1.00 21.00	Ā	N	
ATOM	4287	CA	ASP	556	41.096 55.98		1.00 20.04	Ä	Č	
ATOM	4288	CB	ASP	556	41.500 56.15		1.00 20.02	A	Č	
ATOM	4289	CG	ASP	556	42.649 55.25		1.00 19.76	A	Č	
ATOM	4290	0D1	ASP	556	42.723 54.13		1.00 19.65	A	Ō	
ATOM	4291	0D2	ASP	556	43.470 55.66		1.00 21.90	Α	0	
ATOM	4292	C	ASP	5 56	40.478 54.60		1.00 20.18	Α	C	
ATOM	4293	0	ASP	556	40.856 53.87	4 47. 523	1.00 19.93	A	0	
ATOM	4294	N	THR	557	39. 542 54. 24		1.00 20.55	Α	N	
ATOM	4295	CA	THR	557	38.835 52.96		1.00 22.31	Α	C	
ATOM	4296	CB	THR	557	37. 331 53. 15	4 45.578	1.00 21.37	A	Ċ	
ATOM	4297		THR	557	37.130 53.58	0 44. 224	1.00 21.50	Α	0	
ATOM	4298	CG2		557	36. 754 54. 20	1 46.523	1.00 21:28	Α	С	
ATOM	4299	C	THR	557	39. 294 51. 89	8 44.826	1.00 23.72	Α	С	
ATOM	4300	0	THR	557	38.606 50.89	1 44.633	1.00 25.32	Α	0	
ATOM	4301	N	VAL	558	40. 441 52. 10	5 44.194	1.00 22.84	Α	N	
ATOM	4302	CA	VAL	558	40.931 51.14	3 43. 219	1.00 22.53	Α	C	
ATOM	4303	CB	VAL	558	41.970 51.80	2 42. 294	1.00 22.67	Α	C	
ATOM	4304		VAL	558	42.540 , 50.78	3 41.323	1.00 19.20	A	C	
ATOM	4305		VAL	558	41.323 52.96		1.00 21.12	Α	C	
ATOM	4306	C	VAL	558	41.544 49.90		1.00 23.92	Α	C	
ATOM	4307	0	VAL	558	42.246 50.00		1.00 23.71	Α.	0	
ATOM	4308	N	PHE	559	41. 261 48. 73		1.00 25.05	Α	N	
ATOM	4309	CA	PHE	559	41.815 47.49		1.00 25.45	Α	C	
ATOM	4310	CB	PHE	559	40.855 46.32		1.00 24.60	Α	C	
ATOM	4311	CG	PHE	559	41.476 44.97	7 43. 808	1.00 24.75	Α	C	

					FΙ	G. 4	- 89			(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	4312 4313 4314 4315 4316 4317 4318 4319 4320 4321 4322 4323 4324	CD:	PHE PHE PHE PHE PHE ARG ARG ARG ARG ARG	559	42. 192 41. 382 42. 810 41. 995 42. 709 43. 158 43. 250 44. 188 45. 508 46. 398 45. 869 46. 885 46. 269	44. 352 44. 352 43. 118 43. 125 42. 507 47. 210 47. 246 46. 912 46. 644 47. 892 49. 140 50. 285 51. 536	42. 799 45. 044 43. 021 45. 276 44. 266 43. 170 41. 943 43. 962 43. 397 43. 510	1. 00 25. 70 1. 00 25. 27 1. 00 28. 04 1. 00 24. 71 1. 00 26. 38 1. 00 26. 14 1. 00 27. 21 1. 00 23. 52 1. 00 20. 68 1. 00 19. 21 1. 00 20. 38	A A A A A A A A	C C C C C C O N C C C
ATOM ATOM ATOM ATOM ATOM ATOM	4325 4326 4327 4328 4329 4330	CZ NH1	ARG	560 560 560 560 560 561	45. 637 45. 543 45. 061 46. 274 46. 112 47. 111	51. 536 52. 391 52. 149 53. 468 45. 451 45. 081 44. 856	43. 310 42. 515 41. 218 43. 022 43. 980 45. 145 43. 136	1.00 20.38 1.00 20.51 1.00 26.51 1.00 20.25 1.00 24.37 1.00 24.84 1.00 23.62	A A A A A A	N C N N C O N
ATOM ATOM ATOM ATOM ATOM	4331 4332 4333 4334 4335 4336	CA CB CG CD1 CD2 C	LEU LEU LEU LEU LEU LEU	561 561 561 561 561	47. 968 47. 680 46. 283 46. 139 46. 045 49. 380	43. 740 42. 523 41. 916 40. 749 41. 460 44. 255	43. 511 42. 635 42. 773 41. 803 44. 203 43. 246	1.00 20.95 1.00 18.87 1.00 20.60 1.00 19.75 1.00 17.53 1.00 20.00	A A A A A	C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	4337 4338 4339 4340 4341 4342 4343		LEU ASN ASN ASN ASN ASN	561 562 562 562 562 562 562	49. 894 49. 999 51. 335 51. 197 50. 364 49. 881 50. 195	44. 152 44. 822 45. 392 46. 907 47. 491 48. 610 46. 729	42. 133 44. 274 44. 142 44. 028 45. 148 45. 054	1.00 20.19 1.00 18.97 1.00 18.20 1.00 16.72 1.00 17.45 1.00 19.63	A A A A	0 N C C C O
ATOM ATOM ATOM ATOM ATOM ATOM	4344 4345 4346 4347 4348 4349	C O N CA CB CG	ASN ASN TRP TRP TRP TRP	562 562 563 563 563 563	52. 291 52. 055 53. 375 54. 366 55. 538 56. 741	45. 035 44. 098 45. 793 45. 548 46. 537 46. 249	46. 223 45. 289 46. 056 45. 400 46. 434 46. 290 47. 178	1. 00 18. 39 1. 00 18. 48 1. 00 19. 79 1. 00 17. 98 1. 00 17. 62 1. 00 16. 04 1. 00 15. 76	A A A A A	N C O N C C C
ATOM ATOM ATOM ATOM ATOM	4350 4351 4352 4353 4354 4355	CE2 CE3 CD1 NE1 CZ2	TRP TRP	563 563 563 563 563	57. 474 58. 526 57. 341 57. 367 58. 440 59. 439	47. 200 46. 500 48. 575 45. 041 45. 189 47. 128	47. 968 48. 602 48. 198 47. 361 48. 217 49. 453	1. 00 13. 80 1. 00 11. 13 1. 00 13. 46 1. 00 12. 65 1. 00 11. 34 1. 00 14. 40	A A A A A	C C C C N C
ATOM ATOM ATOM ATOM ATOM		CZ3 CH2 C O N		563 563 563 563 564	58. 252 59. 291 53. 728 54. 048 52. 813	49. 204 48. 476 45. 672 44. 910 46. 620	49. 046 49. 664 47. 809 48. 720 47. 953	1. 00 16. 29 1. 00 14. 18 1. 00 17. 48 1. 00 18. 93 1. 00 16. 80	A A A A	C C C O N

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										(Continued)
•					FΙ	G. 4	- 9 0			
ATOM	4361	CA	ALA	564	52. 151	46.838	49. 232	1.00 17.11	A	С
ATOM	4362	CB	ALA	564	51. 248	48.068	49. 153	1.00 16.72	A	Č
ATOM	4363	C	ALA	564	51.341	45.616	49.655	1.00 17.89	Α	С
ATOM	4364	0	ALA	564	51.322	45.256	50.834	1.00 15.94	Α	0
ATOM	4365	N	THR	565	50.676	44.983	48.691	1.00 18.77	Α	N
ATOM	4366	CA	THR	565	49.870	43.801	48.977	1.00 19.59	Α	C
ATOM	4367	CB	THR	565	49. 368	43. 131	47. 689	1.00 20.01	Α	С
ATOM	4368	0G1		565	48.606	44.069	46. 922	1.00 19.76	Α	0
ATOM	4369		THR	565	48. 496	41.922	48. 027	1.00 19.34	Α	C
ATOM	4370	C	THR	565	50. 718	42. 793	49. 739	1.00 21.27	A	C
ATOM	4371	0	THR	565	50. 290	42. 252	50.760	1.00 22.29	A	0
ATOM	4372	N	TYR	566	51.924	42. 548	49. 234	1.00 22.25	A	N
ATOM	4373	CA	TYR	566	52. 848	41.615	49.864	1.00 23.40	A	C
ATOM	4374	CB	TYR	566	54. 029	41.324	48. 923	1.00 25.18	A	C
ATOM	4375	CCD1	TYR	566	55. 369	41.218	49.616	1.00 25.40	A	C
ATOM	4376		TYR	566	56. 297	42. 262	49.547	1.00 25.62	A	C
ATOM ATOM	4377 4378		TYR TYR	566 566	57. 513	42. 196	50. 226	1.00 26.85	A	C
ATOM	4379		TYR	566	55. 690 56. 903	40. 101	50.382	1.00 26.99	Α .	C
ATOM	4380	CZ	TYR	566	57. 809	40. 023 41. 074	51.073 50.991	1.00 29.74 1.00 30.16	A	C
ATOM	4381	OH	TYR	566	58. 997	40.998	51.688	1.00 30.10	A	C
ATOM	4382	C	TYR	566	53. 369	42.116	51. 212	1.00 32.01	A A	0 C
ATOM	4383	ŏ	TYR	566	53. 458	41.350	52. 170	1.00 23.00	A	0
ATOM	4384	Ň	LEU	567	53. 716	43. 396	51.288	1.00 23.28	A	N N
ATOM	4385	CA	LEU	567	54. 237	43. 949	52. 532	1.00 24.50	A	Č
ATOM	4386	CB	LEU	567	54. 588	45. 429	52. 359	1.00 22.74	Ä	č
ATOM	4387		LEU	567	55. 717	45.769	51.378	1.00 23.15	Ä	č
ATOM	4388		LEU	567	55. 833	47.279	51.263	1.00 20.37	Ä	č
ATOM	4389		LEU	567	57. 038	45.158	51.850	1.00 21.42	A	Č
ATOM	4390	C	LEU	567	53. 243	43.786	53.675	1.00 26.32	Ā	Č
ATOM	4391	0	LEU	567	53.635	43.595	54.824	1.00 27.44	A	Ŏ
ATOM	4392	N	ALA	568	51.955	43.857	53.361	1.00 26.96	Α	N
ATOM	4393	CA	ALA	568	50. 930	43.712	54.383	1.00 27.44	Α	C
ATOM	4394	CB	ALA	568	49. 684	44. 481	53. 984	1.00 26.54	Α	C
ATOM	4395	C	ALA	568	50. 584	42. 242	54.606	1.00 29.12	Α	C
ATOM	4396	0	ALA	568	50. 483	41.782	55. 748	1.00 28.80	Α	0
ATOM	4397	N	SER	569	50. 417	41.506	53.509	1.00 28.58	A	N
ATOM	4398	CA	SER	569	50.062	40.094	53.586	1.00 28.31	A	C
ATOM	4399	CB	SER	569	49. 750	39. 553	52. 191	1.00 28.85	A	Ç
ATOM	4400	OG C	SER	569	49. 420	38. 174	52. 247	1.00 30.69	A	0
ATOM	4401	C	SER	569	51.110	39. 204	54. 236	1.00 27.43	A	C
ATOM ATOM	4402 4403	O N	SER THR	569	50. 800	38. 427	55. 133	1.00 28.44	A	0
ATOM	4403	CA	THR	570 570	52. 350 52. 420	39.311	53. 781	1.00 27.24	A	N
ATOM	4404	CB	THR	570 570	53. 420	38. 483	54.314	1.00 27.02	A	C
ATOM	4406	0G1	THR	570 570	54. 410 53. 749	38. 094 37. 250	53. 199 52. 248	1.00 26.90 1.00 27.63	A	C
ATOM	4407	CG2	THR	570 570	55. 611	37. 369	52. 248 53. 774	1.00 27.03	A A	0 C
ATOM	4408	C	THR	570	54. 203	39.110	55. 459	1.00 23.88	A	C
ATOM	4409	ŏ	THR	570	54. 362	38. 496	56. 512	1.00 27.04	A	0
										-

				FIG. 4-91	(Continued)
ATOM	4410		571	54. 686 40. 329 55. 253 1. 00 26. 71 A	N
ATOM	4411			55. 480 41. 020 56. 259 1. 00 25. 23 A	Č
ATOM	4412			56. 402 42. 040 55. 583 1. 00 24. 64 A	č
ATOM	4413			57. 287 41. 472 54. 473 1. 00 25. 43 A	Č
ATOM	4414			58. 238 40. 392 54. 966 1. 00 27. 45 A	C
ATOM	4415			58. 582 40. 421 56. 164 1. 00 28. 11 A	0
ATOM	4416			58. 656 39. 527 54. 158 1. 00 27. 18 A	0
ATOM	4417			54. 643 41. 715 57. 329 1. 00 24. 50 A	C
ATOM	4418			55. 188 42. 368 58. 213 1. 00 24. 29 A	0
ATOM	4419			53. 324 41. 576 57. 247 1. 00 24. 39 A	N
ATOM ATOM	4420 4421	CA ASN		52. 425 42. 191 58. 223 1. 00 24. 96 A	C
ATOM	4422	CB ASN CG ASN		52. 557 41. 486 59. 569 1. 00 25. 44 A	C
ATOM	4423	OD1 ASN	572	52.139 40.033 59.507 1.00 29.03 A 52.711 39.187 60.192 1.00 30.88 A	C
ATOM	4424	ND2 ASN		E1 100 00 E01 E0 +	0
ATOM	4425	C ASN		E0 000 10 001 T0 110	N
ATOM	4426	0 ASN			C
ATOM	4427	N ILE		52. 642 44. 178 59. 545 1. 00 25. 55 A 52. 944 44. 387 57. 321 1. 00 25. 48 A	0 N
ATOM	4428	CA ILE		53. 208 45. 824 57. 360 1. 00 24. 87 A	N C
ATOM	4429	CB ILE	573	54. 396 46. 198 56. 446 1. 00 24. 59 A	C
ATOM	4430	CG2 ILE	573	54.715 47.669 56.584 1.00 22.90 A	C C C C
ATOM	4431	CG1 ILE	573	55. 622 45. 365 56. 800 1. 00 25. 08 A	č
ATOM	4432	CD1 ILE	573	56.805 45.636 55.900 1.00 25.36 A	Č
ATOM	4433	C ILE	573	51.992 46.621 56.875 1.00 25.22 A	Ċ
ATOM	4434	0 ILE	573	51. 353 46. 249 55. 891 1. 00 24. 86 A	0
ATOM	4435	N ILE	574	51. 681 47. 718 57. 557 1. 00 24. 59 A	N
ATOM ATOM	4436	CA ILE	574	50.557 48.555 57.159 1.00 26.14 A	C
ATOM	4437 4438	CB ILE	574	49. 926 49. 297 58. 359 1. 00 25. 88 A	C
ATOM	4439	CG2 ILE	574	48. 798 50. 190 57. 874 1. 00 26. 06 A	C
ATOM	4440	CD1 ILE	574 574	49. 399 48. 304 59. 386 1. 00 27. 36 A	C
ATOM	4441	CDI ILE	574 574	48. 794 48. 968 60. 607 1. 00 29. 19 A 51. 064 49. 619 56. 191 1. 00 27. 12 A	C
ATOM	4442	0 ILE	574	E4 #00 #0 #04 #0	C
ATOM	4443	N VAL	575	FO 000 10 FO1 F1	0
ATOM	4444	CA VAL	575	50. 683 49. 521 54. 924 1. 00 25. 92 A 51. 128 50. 517 53. 962 1. 00 24. 87 A	N C
ATOM	4445	CB VAL	575	51. 387 49. 904 52. 569 1. 00 24. 76 A	C
ATOM	4446	CG1 VAL	575	51. 973 50. 966 51. 644 1. 00 20. 17 A	Č
ATOM	4447	CG2 VAL	575	52. 320 48. 707 52. 690 1. 00 22. 12 A	č
ATOM	4448	C VAL	575	50.054 51.585 53.837 1.00 25.21 A	č
ATOM	4449	0 VAL	575	48. 929 51. 312 53. 405 1. 00 25. 63 A	Ŏ
ATOM	4450	N ALA	576	50. 403 52. 804 54. 216 1. 00 23. 75 A	Ň
ATOM	4451	CA ALA	576	49. 456 53. 893 54. 152 1. 00 23. 56 A	Ċ
ATOM	4452	CB ALA	576	49. 255 54. 477 55. 540 1. 00 23. 43 A	Ċ
ATOM	4453	C ALA	576	49. 879 54. 988 53. 180 1. 00 24. 06 A	C
ATOM ATOM	4454	O ALA	576	51. 056 55. 139 52. 860 1. 00 22. 16 A	0
ATOM	4455 4456	N SER	577	48. 888 55. 740 52. 710 1. 00 24. 49 A	N
ATOM	4450 4457	CA SER CB SER	577 577	49. 095 56. 852 51. 796 1. 00 23. 11 A	C
ATOM	4458	CB SER OG SER	577 577	48. 793 56. 428 50. 362 1. 00 23. 06 A	C
HIVI	TTUU	NG OUN	577	49. 750 55. 475 49. 921 1. 00 22. 88 A	0

					FI	G. 4	- 92			(Con	tinued)
ATOM	4459	С	SER	577	48. 149	57. 947	52. 248	1.00 22.90	A	С	
ATOM	4460	0	SER	577	47.075		52.768		A	Ō	
ATOM	4461	N	PHE	578	48.546	59.196	52.046	1.00 23.49	· A	N	
ATOM	4462	CA	PHE	578	47.748	60.337	52.479	1.00 21.77	A	С	
ATOM	4463	CB	PHE	578	48. 313		53.804	1.00 21.41	Α	С	
ATOM	4464	CG	PHE	578	47. 585		54.383	1.00 22.79	Α	С	
ATOM	4465		PHE	578	46. 429		55. 144		Α	C	
ATOM	4466		PHE	578	48.080		54. 209	1.00 19.79	Α	C	
ATOM	4467		PHE	578	45. 783		55. 730	1.00 21.26	Α	C	
ATOM	4468		PHE	578	47. 441	64. 381	54. 790	1.00 20.94	Α	С	
ATOM	4469	CZ	PHE	578	46. 288		55. 556	1.00 20.70	Α	С	
ATOM	4470	C	PHE	578	47. 723		51.480	1.00 21.14	A	C	
ATOM	4471	0	PHE	578	48. 766		50. 973	1.00 21.08	A	0	
ATOM	4472	N	ASP	579	46. 533		51. 212	1.00 19.89	A	N	
ATOM	4473	CA	ASP	579 570	46. 389		50. 302	1.00 18.01	Ą	C	
ATOM ATOM	4474 4475	CB CG	ASP	579 570	45. 191	62.985	49. 371	1.00 17.01	A	C	
ATOM	4476		ASP ASP	579 579	45. 334		48. 455	1.00 21.86	A	C	
ATOM	4477		ASP	579	46. 424 44. 342		47. 873	1.00 22.87	A	0	
ATOM	4478	C	ASP	579	44. 342	61.024 64.474	48. 299	1.00 23.17	A	0	
ATOM	4479	0	ASP	579	45. 103	64. 823	51. 092 51. 493	1.00 18.10 1.00 20.42	A	C	
ATOM	4480	N	GLY	580	47. 306	65. 189	51. 493	1.00 20.42	A	0	
ATOM	4481	CA	GLY	580	47. 238	66.439	52. 044	1.00 17.22	A A	N C	
ATOM	4482	C	GLY	580	47. 065	67.610	51.098	1.00 16.53	A	Č	
ATOM	4483	Ŏ	GLY	580	46.544	67.462	49. 993	1.00 17.18	A	0	
ATOM	4484	N	ARG	581	47. 495	68.786	51.528	1.00 15.90	A	N	
ATOM	4485	CA	ARG	581	47. 377	69.970	50. 701	1.00 15.52	A	C	
ATOM	4486	CB	ARG	581	47.956	71.172	51.444	1.00 16.17	Ä	č	
ATOM	4487	CG	ARG	581	47.072	71.645	52.585	1.00 16.05	Ä	č	
ATOM	4488	CD	ARG	581	47. 756	72.653	53.467	1.00 14.87	Ä	Č	
ATOM	4489	NE	ARG	581	48.617	71.990	54. 441	1.00 18.25	Ä	Ň	
ATOM	4490	CZ	ARG	581	49. 321	72.624	55.375	1.00 19.44	Ä	Ċ	
ATOM	4491		ARG	581	49. 268	73.952	55.463	1.00 20.41	A	Ň	
ATOM	4492		ARG	581	50. 075	71.933	56. 224	1.00 15.76	Α	N	
ATOM	4493	C	ARG	581	48. 107	69. 742	49. 386	1.00 17.75	Α	C	
ATOM	4494	0	ARG	581	49. 193	69.158	49. 357	1.00 17.49	Α	0	
ATOM	4495	N	GLY	582	47. 495	70. 192	48. 295	1.00 18.96	Α	N	
ATOM	4496	CA	GLY	582	48. 094	70.022	46. 987	1.00 17.63	Α	. C	
ATOM	4497	C	GLY	582	47. 511	68.842	46. 231	1.00 18.54	A	C	
ATOM ATOM	4498	0 N	GLY	582	47. 673	68.757	45.017	1.00 18.99	A	0	
ATOM	4499 4500	N CA	SER SER	583	46.842	67. 923	46. 925	1.00 18.00	A	N	
ATOM	4500 4501	CB	SER	583 583	46. 258	66.765	46. 247	1.00 18.46	A	C	
ATOM	4502	OG	SER	583	45.842	65.700	47. 269	1.00 18.34	A	C	
ATOM	4502	C	SER	583	45. 058 45. 068	66. 253	48. 303	1.00 19.12	A	0	
ATOM	4504	0	SER	583	40.008 44.601	67. 218 68. 344	45. 392	1.00 18.03	A	C	
ATOM	4505	N	GLY	584	44. 570	66. 355	45. 536 44. 510	1.00 17.42	A	0 N	
ATOM	4506	CA	GLY	584	43. 481	66. 779	44. 510	1.00 17.84 1.00 19.22	A	N	
ATOM	4507	C	GLY	584	42. 052	66. 293	43. 827	1.00 19.22	A A	C C	
	2001	v	J. 1	001	T4. VU4	00.400	40.041	1.00 13.43	Α	U	

•			FIG. 4-93	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	4509 N TY 4510 CA TY 4511 CB TY 4512 CG TY 4513 CD1 TY 4514 CE1 TY 4515 CD2 TY 4516 CE2 TY 4517 CZ TY 4518 OH TY 4519 C TY 4519 C TY 4520 O TY 4521 N GLI 4522 CA GLI 4523 CB GLM 4524 CG GLM 4525 CD GLM 4526 OE1 GLM 4527 NE2 GLM	R 585 R 586	41. 724 65. 570 44. 767 1. 00 21. 57 41. 191 66. 735 42. 917 1. 00 19. 76 39. 782 66. 362 42. 906 1. 00 18. 53 39. 673 64. 859 42. 663 1. 00 18. 57 40. 578 64. 401 41. 550 1. 00 18. 83 40. 439 64. 914 40. 260 1. 00 19. 48 41. 300 64. 533 39. 235 1. 00 18. 11 41. 606 63. 490 41. 789 1. 00 19. 81 42. 476 63. 100 40. 769 1. 00 17. 71 42. 313 63. 626 39. 497 1. 00 18. 76 43. 150 63. 232 38. 481 1. 00 20. 70 38. 997 66. 751 44. 152 1. 00 18. 81 38. 046 66. 067 44. 521 1. 00 17. 85 39. 382 67. 861 44. 783 1. 00 20. 25 38. 708 68. 345 45. 986 1. 00 20. 04 39. 455 67. 886 47. 233 1. 00 20. 09 39. 770 66. 412 47. 279 1. 00 20. 60 40. 781 66. 095 48. 363 1. 00 24. 77 40. 441 66. 029 49. 548 1. 00 23. 60 42. 044 65. 919 47. 962 1. 00 25. 12	(Continued) 0 N C C C C C C C C C C C C C C C C C
ATOM	4528 C GLN 4529 O GLN		38. 619 69. 869 46. 024 1. 00 22. 06 A	С
ATOM	4530 N GLY		20 702 70 510 44 077 1 00 01 7	0
ATOM	4531 CA GLY	587	38. 707 71. 969 44. 853 1. 00 21. 79 A	N C
ATOM	4532 C GLY		40. 073 72. 623 44. 883 1. 00 21. 56 A	C C
ATOM	4533 O GLY		41.033 72.035 45.364 1.00 23.11 A	0
ATOM	4534 N ASP	_	40.154 73.856 44.397 1.00 21.25 A	N
ATOM ATOM	4535 CA ASP	588	41.415 74.580 44.339 1.00 22.09 A	č
ATOM	4536 CB ASP 4537 CG ASP	588	41. 287 75. 763 43. 382 1. 00 22. 35 A	č
ATOM	4537 CG ASP 4538 OD1 ASP	588 500	40. 944 75. 340 41. 965 1. 00 25. 14 A	C
ATOM	4539 OD2 ASP	588 588	40. 465 76. 213 41. 211 1. 00 25. 77 A	0
ATOM	4540 C ASP	588	41. 157 74. 155 41. 599 1. 00 24. 41 A 41. 955 75. 079 45. 675 1. 00 23. 08 A	0
ATOM	4541 0 ASP	588	12.000 10.013 40.013 1.00 23.08 A	C
ATOM	4542 N LYS	589	41 190 75 000 to 510	0
ATOM	4543 CA LYS	589		IX C
ATOM	4544 CB LYS	589	40. 509 75. 616 49. 037 1. 00 22. 97 A	C C
ATOM	4545 CG LYS	589	40. 994 76. 173 50. 365 1. 00 29. 68 A	Č
ATOM ATOM	4546 CD LYS	589	39. 916 76. 141 51. 439 1. 00 35. 08 A	č
ATOM	4547 CE LYS 4548 NZ LYS	589	40. 457 76. 638 52. 784 1. 00 36. 09 A	Č
ATOM	4549 C LYS	589 589	39. 461 76. 464 53. 881 1. 00 36. 83 A	N
ATOM	4550 0 LYS	589	42.705 74.611 48.468 1.00 22.93 A 43.711 75.032 49.033 1.00 23.71	C
ATOM	4551 N ILE	590	49 404 79 996 49 947 1 3 3 3 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	0
ATOM	4552 CA ILE	· 590	42 444 79 909 40 907 1 99 71	N ·
ATOM	4553 CB ILE	590	43. 444	C
ATOM	4554 CG2 ILE	590	43. 756 69. 841 48. 934 1. 00 19. 40 A	C
ATOM	4555 CG1 ILE	590	41.901 71.025 50.126 1.00 21.94 A	Č
ATOM	4556 CD1 ILE	590	41. 200 69. 720 50. 478 1. 00 22. 22 A	č

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					FΙ	G. 4	- 94			(Continued)
ATOM	4557	С	ILE	590	44. 537		47. 562	1.00 22.32	٨	С
ATOM	4558	ŏ	ILE	590	45. 711		47. 901	1.00 22.52	A A	0
ATOM	4559	N	MET	591	44. 157		46. 291	1.00 21.59	A	N N
ATOM	4560	CA	MET	591	45. 127	71.846	45. 232	1.00 21.59	A	C
ATOM	4561	CB	MET	591	44. 406		43. 917	1.00 21.80	A	č
ATOM	4562	CG	MET	591	45. 309		42. 838	1.00 21.85	Ä	č
ATOM	4563	SD	MET	591	44. 403		41.309	1.00 22.76	Ä	Š
ATOM	4564	CE	MET	591	44. 237		40. 732	1.00 22.84	A	č
ATOM	4565	C	MET	591	46. 112		45.051	1.00 21.43	A	Č
ATOM	4566	0	MET	591	47. 289		44. 791	1.00 19.25	A	0
ATOM	4567	N	HIS	592	45.636		45. 200	1.00 21.21	Ā	N
ATOM	4568	CA	HIS	592	46.502		45: 035	1.00 21.43	Α	C
ATOM	4569	CB	HIS	592	45.713	76.560	44.455	1.00 22.32	Α	C
ATOM	4570		HIS	592	45. 296	76.361	43.032	1.00 24.65	Α	C
ATOM	4571		HIS	592	45.604		42.139	1.00 26.25	A	C
ATOM	4572		HIS	592	44. 471		42.368	1.00 25.75	A	N
ATOM	4573		HIS	592	44. 289		41.128	1.00 25.99	A	C
ATOM	4574		HIS	592	44.965		40.962	1.00 25.78	Α	N
ATOM	4575	C	HIS	592	47.197		46.319	1.00 21.38	Α	C
ATOM	4576	0	HIS	592	47.842		46.362	1.00 20.84	Α	0
ATOM	4577	N	ALA	593	47.076		47. 367	1.00 21.76	· A	N
ATOM	4578	CA	ALA	593	47. 732		48. 628	1.00 20.43	A	C
ATOM	4579	CB	ALA	593	47. 360		49.710	1.00 18.24	A	C
ATOM	4580	C	ALA	593	49. 241	75.361	48. 427	1.00 19.92	A	C
ATOM ATOM	4581	0 N	ALA	593	49. 940	76.126	49.081	1.00 21.91	A	0
ATOM	4582 4583	N CA	ILE	594 504	49. 736	74. 522	47.518	1.00 19.47	A	N
ATOM	4584	CB	ILE ILE	594 594	51.176	74. 446	47. 248	1.00 20.49	A	C
ATOM	4585		ILE	594 594	51.617 51.467	73. 021 72. 051	46. 816 47. 966	1.00 19.36	A	C
ATOM	4586		ILE	594	50. 814	72. 581	45. 590	1.00 19.38 1.00 21.33	A	C
ATOM	4587		ILE	594	50. 951	71. 106	45. 243	1.00 21.33	A A	C C
ATOM	4588	C	ILE	594	51.658	75. 410	46. 169	1.00 19.88	A	C
ATOM	4589	ŏ	ILE	594	52. 849	75. 434	45.854	1.00 17.79	A	0
ATOM	4590	Ň	ASN	595	50. 746	76. 200	45.606	1.00 20.03	A	N
ATOM	4591	CA	ASN	595	51.119	77. 137	44. 547	1.00 21.76	Ä	Č
ATOM	4592	CB	ASN	595	49. 977	78. 114	44. 265	1.00 20.68	Ä	č
ATOM	4593	CG	ASN	595	50. 300	79.072	43.128	1.00 21.80	Ä	č
ATOM	4594	0D1	ASN	595	50.640	78.652	42.024	1.00 22.78	Ä	Ö
ATOM	4595	ND2	ASN	595	50.191	80.364	43.394	1.00 22.74	Ā	N
ATOM	4596	С	ASN	595	52. 395	77.921	44.860	1.00 22.25	A	Ĉ
ATOM	4597	0	ASN	595	52.442	78.688	45.824	1.00 22.44	Α	0
ATOM	4598	N	ARG	596	53. 421	77.715	44.031	1.00 22.52	Α	N
ATOM	4599	CA	ARG	596	54.726	78. 378	44. 171	1.00 22.41	A	С
ATOM	4600	CB	ARG	596	54. 550	79.898	44. 141	1.00 21.28	Α	C
ATOM	4601	CG	ARG	596	53.894	80.426	42.880	1.00 21.31	Α	C
ATOM	4602	CD	ARG	596	53. 398	81.856	43.096	1.00 22.01	Α	С
ATOM	4603	NE	ARG	596	54. 479	82.760	43. 482	1.00 20.88	Α	N
ATOM	4604	CZ	ARG	596	55. 467	83. 112	42.671	1.00 21.35	A	C
ATOM	4605	NH1	AKG	596	55. 498	82. 635	41.431	1.00 22.62	Α	N

					FΙ	G. 4	- 9 5			(Continued)
ATOM	4606	NH	2 ARG	596	56. 427	83. 924		1.00 19.92	A	N
ATOM	4607		ARG		55. 492	77. 982		1.00 21.53	A	Č
ATOM	4608	0	ARG		56. 482	78.611	45.804	1.00 20.59	A	ŏ
ATOM	4609	N	ARG		55.046	76.930		1.00 21.66	A	N
ATOM	4610	CA	ARG	597	55.705	76.512		1.00 21.98	A	Č
ATOM	4611			597	54.943	77.061	48.539	1.00 23.55	A	č
ATOM	4612			597	55.184	78.547	48.776	1.00 28.20	Ä	č
ATOM	4613				56.611	78.813	49. 264	1.00 30.86	Ä	Č
ATOM	4614				56.891	80.239	49.414	1.00 34.81	Ā	N
ATOM	4615				57. 074	81.088	48. 401	1.00 36.01	A	Č
ATOM	4616		1 ARG		57.011	80.670	47. 142	1.00 33.57	A	N
ATOM	4617		2 ARG		57. 326	82.365	48.650	1.00 37.36	Α	N
ATOM	4618		ARG		55. 869	75.011	47. 458	1.00 20.79	A	C
ATOM	4619		ARG		55. 523	74. 423	48. 487	1.00 20.19	Α	0
ATOM	4620	N	LEU		56.400	74.398	46. 404	1.00 19.44	Α	N
ATOM	4621	CA	LEU	598	56.649	72.963	46. 387	1.00 18.48	Α	C
ATOM	4622	CB	LEU	598	57. 142	72.545	45.003	1.00 18.20	Α	C
ATOM ATOM	4623	CC	LEU	598	56.119	72.007	43. 994	1.00 19.27	Α	C
ATOM	$\begin{array}{c} 4624 \\ 4625 \end{array}$		LEU LEU	598	54. 800	72. 731	44. 107	1.00 19.49	A	C
ATOM	4626	CDZ	LEU	598 598	56. 691	72.135	42. 595	1.00 18.24	A	C
ATOM	4627	0	LEU	598	57. 692 58. 644	72.617	47. 450	1.00 19.10	A	C
ATOM	4628	·N	GLY	599	56. 044 57. 506	73. 363 71. 485	47.679	1.00 19.27	A	0
ATOM	4629	CA	GLY	599	58. 440	71.090	48. 108 49. 138	1.00 19.24	A	N
ATOM	4630	C	GLY	599	58. 055	71.622	50. 508	1.00 20.34 1.00 21.76	A	C
ATOM	4631	Ō	GLY	599	58. 882	71.640	51.422	1.00 21.70	A A	C 0
ATOM	4632	N	THR	600	56. 811	72.061	50. 666	1.00 23.38	A	N N
ATOM	4633	CA	THR	600	56. 381	72. 578	51.958	1.00 21.02	A	C
ATOM	4634	CB	THR	600	56.039	74. 082	51.874	1.00 21.28	A	C
ATOM	4635	0G1	THR	600		74. 271	51.052	1.00 25.68	A	Ö
ATOM	4636	CG2	THR	600	57. 192	74.856	51.264	1.00 21.23	A	Č
ATOM	4637	C	THR	600	55. 201	71.810	52.557	1.00 21.38	A	č
ATOM	4638	0	THR	600	55. 386	70.724	53.100	1.00 22.42	Ä	Ŏ
ATOM	4639	N	PHE	601	53.993	72.356	52.446	1.00 21.18	Ā	Ň
ATOM	4640	CA	PHE	601		71.721	53.022	1.00 22.09	Α	C
ATOM	4641	CB	PHE	601		72.498	52.649	1.00 24.93	A	C
ATOM	4642	CG	PHE	601		73. 935	53.077	1.00 26.21	Α	C
ATOM	4643		PHE	601		74. 923	52. 236	1.00 28.07	Α	C
ATOM ATOM	4644		PHE	601		74. 308		1.00 26.83	Α	C
ATOM	4645 4646		PHE	601		76. 271		1.00 29.10	A	C
ATOM	4647	CZ	PHE PHE	601		75. 650		1.00 28.02	A	C
ATOM	4648	CZ	PHE	601 601		76. 636	53. 830	1.00 28.61	A	Č
ATOM	4649	0	PHE	601		70. 265	52.635	1.00 22.45	A	C
ATOM	4650	N	GLU	602		69. 451		1.00 22.89	A	0
ATOM	4651	CA	GLU	602		69. 931 68. 556		1.00 22.76	A	N ·
ATOM	4652	CB	GLU	602		68. 418		1.00 21.82	A	C
ATOM	4653	CG	GLU	602		68. 559		1.00 22.43 1.00 27.44	A	C
ATOM	4654	CD	GLU	602		70. 002		1.00 27.44	A A	C C
					- A- O1 B		10.000	1.00 00. [1	Λ	U

			FIG. 4-96	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	4656 OE2 GLU 4657 C GLU 4658 O GLU 4659 N VAI 4660 CA VAI 4661 CB VAI	J 602 J 602 J 603 C 603 C 603 C 603 C 603 C 603 C 604 C 604	F I G. 4 - 96 54.751 70.743 49.891 1.00 31.66 55.379 70.392 47.822 1.00 31.46 53.663 67.657 51.698 1.00 21.67 53.386 66.473 51.899 1.00 20.78 55.772 67.468 52.897 1.00 20.76 57.159 68.133 52.800 1.00 18.99 58.165 67.365 53.649 1.00 15.00 57.603 68.193 51.335 1.00 15.00 57.603 68.193 51.335 1.00 15.21 55.373 66.265 54.946 1.00 20.44 55.009 68.481 54.951 1.00 24.70 54.594 68.518 56.341 1.00 27.84 54.322 69.964 56.770 1.00 30.83 55.572 70.808 56.924 1.00 37.92 56.449 70.355 58.091 1.00 43.63 57.505 70.989 58.328 1.00 46.30 50.083 69.368 58.7	A 0 A 0 A 0 A 0 A 0 A 0 A 0 A 0 A 0 A 0
			CUDCTITUTE CULTET (DUILE 20)	

					FΙ	G. 4	- 9 7			(Continued)
ATOM	4704	CD	GLU	608	50.054	66. 482	62. 389	1.00 38.42	A	С
ATOM	4705	0E1			49. 197	66. 454	63. 302	1.00 37.67	A	Õ
ATOM	4706	0E2			51. 285	66. 435	62. 625	1.00 40.64	Ä	Ö
ATOM	4707	C.	GLU		50.606	63.891	60.012	1.00 32.76	A	Č
ATOM	4708	0	GLU		49.889	63. 527	60.947	1.00 33.47	Ā	0
ATOM	4709	N	ALA		50.643	63.270	58.836	1.00 31.32	A	Ň
ATOM	4710	CA	ALA		49.827	62.090	58. 595	1.00 30.73	A	Ĉ
ATOM	4711	CB	ALA		49.883	61.682	57.123	1.00 28.50	Ā	Č
ATOM	4712	C	ALA		50.355	60.968	59.472	1.00 30.16	A	C C
ATOM	4713	0	ALA		49.583	60.274	60.139	1.00 31.03	Ā	0
ATOM	4714	N	ALA		51.674	60.803	59.479	1.00 29.26	A	N
ATOM	4715	CA	ALA		52.310	59.758	60.274	1.00 28.48	A	C
ATOM	4716	CB	ALA		53.826	59.818	60.114	1.00 27.67	A	C
ATOM	4717	C	ALA	610	51.930	59.886	61.743	1.00 27.62	Α	C
ATOM	4718	0	ALA	610	51.556	58.904	62.379	1.00 28.43	Α	0
ATOM	4719	N	ARG	611	52.025	61.094	62.282	1.00 26.94	Α	N
ATOM		CA	ARG	611	51.674	61.309	63.678	1.00 28.98	Α	C
ATOM	4721	CB	ARG	611	51.812	62.787	64.042	1.00 28.96	Α	C
ATOM	4722	CG	ARG	611	53. 239	63. 291	64.032	1.00 29.26	Α	C
ATOM	4723	CD	ARG	611	53. 281	64. 799	64.187	1.00 29.92	Α	C
ATOM	4724	NE	ARG	611	54.641	65.322	64.102	1.00 28.90	Α	N ·
ATOM	4725	CZ	ARG	611	54.980	66. 384	63.378	1.00 29.97	Α	C
ATOM	4726		ARG	611	54.055	67.028	62.680	1.00 31.41	Α	N
ATOM	4727		ARG	611	56.237	66.802	63.347	1.00 29.57	Α	N
ATOM	4728	C	ARG	611	50. 242	60. 846	63.923	1.00 29.90	Α	С
ATOM	4729	0	ARG	611	49. 983	60. 084	64.856	1.00 31.08	Α	0
ATOM	4730	N	GLN	612	49. 319	61.298	63.076	1.00 30.18	Α	N
ATOM	4731	CA	GLN	612	47.916	60. 922	63.195	1.00 30.42	Α	C
ATOM	4732	CB	GLN	612	47. 108	61.497	62.035	1.00 30.55	A	C
ATOM	4733	CG	GLN	612	47.112	63.001	61.964	1.00 33.70	A	C
ATOM	4734	CD	GLN	612	46. 446	63. 637	63. 162	1.00 34.91	A	C
ATOM	4735		GLN	612	45. 276	63. 379	63. 444	1.00 35.03	A	0
ATOM	4736		GLN	612	47. 188	64. 475	63. 875	1.00 35.30	A	N
ATOM	4737	C	GLN	612	47. 740	59. 405	63. 223	1.00 30.70	A	C
ATOM ATOM	4738 4739	0 N	GLN	612	46. 993	58. 878	64.049	1.00 31.56	A	0
ATOM	4740	N CA	PHE PHE	613	48. 415	58. 698	62.324	1.00 30.50	Ą	N
ATOM	4741	CB		613	48. 291	57. 248	62.301	1.00 32.33	A	C
ATOM	4742	CG	PHE	613	49.043	56.653	61.114	1.00 31.37	A	C
ATOM	4743		PHE PHE	613	48. 537	57. 126	59. 787	1.00 30.49	A	C
ATOM	4744		PHE	613	47. 167	57.171	59. 529	1.00 30.03	A	C
ATOM	4745		PHE	613 613	49. 423 46. 687	57. 523	58. 793	1.00 28.11	A	C
ATOM	4746		PHE	613	48. 954	57. 604 57. 959	58. 300	1.00 29.96 1.00 28.75	A	C
ATOM	4747	CZ	PHE	613	47. 585	58.·001	57. 309	1.00 28.70	A	C
ATOM	4748	C	PHE	613	48.835	56.679	63. 597	1.00 28.70	.Α Λ	C
ATOM	4749	0	PHE	613	48. 327	55. 677	64. 107	1.00 34.28	A A	C 0
ATOM	4750	N	SER	614	49. 865	57. 326	64. 134	1.00 34.47	A	N N
ATOM	4751	CA	SER	614	50. 454	56.884	65. 388	1.00 33.01	A	C
ATOM	4752	CB	SER	614	51.723	57. 677	65. 683	1.00 38.32	A	Č

						~ 4	0.0			(Continued)
				* -4*	FΙ	G. 4	- 98			
ATOM	4753	0G	SER	614	52. 686	57. 477	64. 663	1.00 38.53	A	0
ATOM	4754	C	SER	614	49. 424	57. 098	66. 494	1.00 39.76		C
ATOM	4755	Õ	SER	614	49. 283	56. 276	67. 398	1.00 39.70	A	
ATOM	4756	N	LYS	615					A	0 N
ATOM	4757	CA	LYS	615	48. 694	58. 204	66. 413	1.00 40.51 1.00 41.32	A	N C
ATOM	4758	CB	LYS	615	47.663	58. 490	67.400		A	C
ATOM	4759	CG	LYS	615	47. 047	59.870	67. 155	1.00 42.73	A	C
ATOM	4760	CD	LYS	615	47. 884	61.040	67. 642 67. 631	1.00 44.59	A	C
ATOM	4761	CE	LYS	615	47.064	62.330		1.00 46.18	A	C
ATOM	4762	NZ	LYS		47. 864	63.511	68. 168	1.00 46.73	A	C
ATOM	4763	C	LYS	615 615	48.314	63. 301	69. 577	1.00 48.03	A	N C
ATOM	4764	0	LYS	615	46. 552	57.441	67. 347	1.00 40.86	A	C
ATOM	4765	N	MET	616	45. 794	57. 285	68. 303	1.00 41.94	A	0
ATOM	4766	CA	MET	616	46. 456	56. 724	66. 230	1.00 39.78 1.00 37.88	A	N
ATOM	4767	CB	MET	616	45. 418	55.712	66.065		A	C
ATOM	4768	CG	MET	616	45. 246 44. 673	55. 374 56. 532	64. 578 63. 768	1.00 37.42	A	C
ATOM	4769	SD	MET	616	44. 195	56. 101	62.079	1.00 35.95 1.00 35.73	A	C
ATOM	4770	CE	MET	616	43. 946	57. 730	61.385	1.00 33.73	A	S C
ATOM	4771	C	MET	616	45. 654	54. 447	66. 885	1.00 34.00	A A	Č
ATOM	4772	ŏ	MET	616	44. 908	53. 473	66. 772	1.00 37.22	A	0
ATOM	4773	N	GLY	617	46. 706	54. 469	67. 698	1.00 37.22	A	N N
ATOM	4774	CA	GLY	617	47. 013	53. 355	68. 578	1.00 33.13	A	C
ATOM	4775	C	GLY	617	47. 445	51.995	68.065	1.00 32.74	A	Č
ATOM	4776	ŏ	GLY	617	47. 806	51.143	68. 872	1.00 33.71	A	Ŏ
ATOM	4777	Ň	PHE	618	47. 409	51.751	66. 761	1.00 32.52	Ä	N
ATOM	4778	CA	PHE	618	47. 841	50.447	66. 262	1.00 31.36	A	Č
ATOM	4779	CB	PHE	618	46. 701	49. 759	65.496	1.00 31.10	Ä	č
ATOM	4780	CG	PHE	618	46.047	50.624	64.457	1.00 31.61	Ä	č
ATOM	4781		PHE	618	46.743	51.025	63. 322	1.00 31.30	Ä	č
ATOM	4782		PHE	618	44.724	51.027	64.607	1.00 30.93	Ä	č
ATOM	4783		PHE	618	46. 129	51.815	62.349	1.00 31.53	Ā	č
ATOM	4784	CE2	PHE	618	44.104	51.814	63.642	1.00 30.94	Ā	Č
ATOM	4785	CZ	PHE	618	44.808	52.209	62.509	1.00 29.86	A	Č
ATOM	4786	C	PHE	618	49. 109	50.521	65.404	1.00 30.95	Α	C
ATOM	4787	0	PHE	618	49.303	49.735	64.477	1.00 30.95	Α	0
ATOM	4788	N	VAL	619	49.982	51.465	65.732	1.00 30.23	Α	N
ATOM	4789	CA	VAL	619	51.226	51.627	64.996	1.00 29.99	Α	C
ATOM	4790	CB	VAL	619	51.226	52.928	64. 147	1.00 29.39	Α	C
ATOM	4791	CG1		619	52.632	53. 200	63.617	1.00 28.74	A	C
ATOM	4792	CG2		619	50. 248	52.804	62.994	1.00 26.48	A	C
ATOM	4793	C	VAL	619	52.425	51.673	65. 931	1.00 29.66	Α	C
ATOM	4794	0	VAL	619	52.400	52.342	66.962	1.00 30.05	Α	0
ATOM	4795	N	ASP	620	53. 475	50. 954	65. 561	1.00 29.84	A	N
ATOM	4796	CA	ASP	620	54. 695	50. 932	66.347	1.00 29.07	A	C
ATOM	4797	CB	ASP	620	55. 563	49. 748	65. 924	1.00 27.94	A	C
ATOM	4798	CG	ASP	620	56. 789	49. 587	66. 794	1.00 27.02	A	C
ATOM	4799	0D1		620	57. 191	50. 580	67.439	1.00 26.38	A	0
ATOM	4800	0D2		620	57. 358	48. 473	66.818	1.00 25.22	A	0
ATOM	4801	C	ASP	620	55. 408	52. 243	66.039	1.00 30.30	A	С

					FIG. 4-99	(Continued)
ATOM	4802		ASP	620	56.009 52.398 64.979 1.00 29.95 A	0
ATOM	4803		ASN	621	55. 330 53. 196 66. 958 1. 00 33. 01 A	N
ATOM	4804			621	55. 962 54. 492 66. 746 1. 00 35. 15 A	C
ATOM	4805		ASN	621	55.761 55.376 67.975 1.00 38.29 A	C
ATOM	4806			621	56. 420 54. 804 69. 214 1. 00 43. 03 A	С
ATOM	4807		I ASN	621	57. 648 54. 821 69. 346 1. 00 44. 79 A	0
ATOM	4808		2 ASN	621	55. 606 54. 280 70. 130 1. 00 45. 61 A	N
ATOM	4809		ASN	621	57. 453 54. 370 66. 441 1. 00 35. 20 A	С
ATOM	4810		ASN	621	58. 083 55. 330 66. 004 1. 00 34. 67 A	0
ATOM ATOM	4811	N	LYS	622	58. 016 53. 186 66. 660 1. 00 36. 30 A	N
ATOM	4812 4813	CA	LYS	622	59. 439 52. 977 66. 418 1. 00 35. 70 A	C
ATOM	4814	CB CG	LYS	622	60.030 52.027 67.464 1.00 37.42 A	C
ATOM	4815	CD	LYS LYS	$622 \\ 622$	60. 148 52. 611 68. 866 1. 00 39. 14 A	C
ATOM	4816	CE	LYS	622	60. 763 51. 584 69. 804 1. 00 43. 05 A 60. 839 52. 077 71. 240 1. 00 45. 27 A	C
ATOM	4817	NZ	LYS	622	01 F10 F1 0FF F0 100	C
ATOM	4818	C	LYS	622	FO MAO HO 11	N
ATOM	4819	ŏ	LYS	622	40 004 50 550	C
ATOM	4820	Ň	ARG	623	FO FOR P4 040	0 N
ATOM	4821	CA	ARG	623	EO 000 E4 000 00 000	N C
ATOM	4822	CB	ARG	623	59. 030 51. 308 63. 046 1. 00 29. 60 A 58. 821 49. 791 63. 058 1. 00 29. 94 A	C C
ATOM	4823	CG	ARG	623	59. 767 49. 071 64. 009 1. 00 32. 12 A	Č
ATOM	4824	CD	ARG	623	59. 117 47. 832 64. 614 1. 00 33. 42 A	C
ATOM	4825	NE	ARG	623	59. 247 46. 663 63. 758 1. 00 34. 25 A	N
ATOM	4826	CZ	ARG	623	58. 457 45. 601 63. 833 1. 00 34. 36 A	Č
ATOM	4827		ARG	623	57.476 45.572 64.725 1.00 35.41 A	Ň
ATOM	4828		ARG	623	58. 655 44. 571 63. 021 1. 00 33. 15 A	Ň
ATOM	4829	C	ARG	623	58.179 51.957 61.962 1.00 27.66 A	Ċ
ATOM	4830	0	ARG	623	57. 315 51. 313 61. 363 1. 00 27. 44 A	0
ATOM	4831	N	ILE	624	58. 425 53. 241 61. 720 1. 00 25. 16 A	N
ATOM	4832	CÁ	ILE	624	57. 708 53. 977 60. 685 1. 00 24. 70 A	C
ATOM	4833	CB	ILE	624	57. 114 55. 298 61. 224 1. 00 24. 52 A	C
ATOM ATOM	4834 4835	CC1	ILE	624	56. 391 56. 025 60. 107 1. 00 23. 47 A	C
ATOM	4836		ILE	624	56. 136 55. 021 62. 371 1. 00 24. 01 A	C
ATOM	4837	CDI	ILE ILE	624	55. 473 56. 277 62. 936 1. 00 19. 15 A	C
ATOM	4838	0	ILE	624 624	58. 667 54. 311 59. 532 1. 00 24. 37 A	C
ATOM	4839	N	ALA	625	59. 651 55. 034 59. 709 1. 00 23. 38 A	0
ATOM	4840	CA	ALA	625	58. 384 53. 768 58. 356 1. 00 22. 58 A 59. 213 54. 014 57. 189 1. 00 21. 00 A	N .
ATOM	4841	CB	ALA	625	FO CTO FO COO FO FOO A CO CO	C
ATOM	4842	C	ALA	625	FO 400 F4 000 F6 400 4 00 04 00	C
ATOM	4843	ŏ	ALA	625	57 900 F4 900 F0 95F 4 99 94 95	C
ATOM	4844	Ň	ILE	626	FO 10F FF 00F FF 10F 1 00 15 00	0
ATOM	4845	CA	ILE	626	FO FOO FO 150 51 105 1 00 10 50	N C
ATOM	4846	CB	ILE	626	58. 502 56. 178 54. 137 1. 00 18. 63 A 58. 589 57. 699 54. 446 1. 00 18. 98 A	C
ATOM	4847	CG2		626	60. 032 58. 103 54. 694 1. 00 18. 36 A	C C
ATOM	4848	CG1	ILE	626	57. 973 58. 501 53. 296 1. 00 19. 11 A	C
ATOM	4849	CD1		626	57.872 59.991 53.562 1.00 18.34 A	C
ATOM	4850	C	ILE	626	59. 185 55. 882 52. 809 1. 00 17. 48 A	Č

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					FIG	. 4 -	100			(Continued)
ATOM	4851	0	ILE	626	60.380	55.619	52.776	1.00 17.10	A	0
ATOM	4852	N	TRP	627	58. 425	55.893	51.719	1.00 17.62	Ā	N
ATOM	4853	CA	TRP	627	58. 998	55.622	50.409	1.00 17.62	Ā	Ċ
ATOM	4854	CB	TRP	627	59. 190	54.118	50.206	1.00 16.80	Ā	Č
ATOM	4855	CG	TRP	627	58.096	53.441	49.427	1.00 18.70	A	Č
ATOM	4856	CD2		627	58. 139	53.055	48.044	1.00 17.58	A	Č
ATOM	4857	CE2		627	56.912	52.425	47.749	1.00 17.70	A	C
ATOM	4858	CE3		627	59.095	53.179	47.028	1.00 15.10	A	C
ATOM	4859	CD1		627	56.879	53.047	49.895	1.00 18.68	Α	C
ATOM	4860	NE1	TRP	627	56.163	52.435	48.896	1.00 18.72	A	N
ATOM	4861	CZ2	TRP	627	56.617	51.916	46.480	1.00 16.42	A	С
ATOM	4862	CZ3		627	58.801	52.673	45.769	1.00 14.48	A	C
ATOM	4863	CH2	TRP	627	57. 575	52.048	45.507	1.00 14.63	Α	C
ATOM	4864	C	TRP	627	58. 157	56.191	49.275	1.00 18.48	A	С
ATOM	4865	0	TRP	627	56.934	56.280	49. 381	1.00 18.15	Α	0
ATOM	4866	N	GLY	628	58.829	56.579	48. 193	1.00 18.70	A	N
ATOM	4867	CA	GLY	628	58. 140	57.146	47.049	1.00 18.30	Α	C
ATOM	4868	C	GLY	628	58.986	57.163	45. 787	1.00 18.36	Α	C
ATOM	4869	0	GLY	628	60. 212	57.065	45. 833	1.00 19.07	A	0
ATOM	4870	N	TRP	629	58. 312	57.300	44.654	1.00 17.25	Α	N
ATOM	4871	CA	TRP	629	58. 945	57. 322	43. 343	1.00 15.27	A	C
ATOM	4872	CB	TRP	629	58. 306	56. 214	42. 494	1.00 10.48	A	C
ATOM	4873	CG	TRP	629	59. 131	55.698	41.357	1.00 10.84	A	C
ATOM	4874		TRP	629	59.512	54. 335	41.122	1.00 9.02	A	C
ATOM	4875		TRP	629	60. 243	54.310	39. 914	1.00 10.87	A	C
ATOM ATOM	4876 4877	CD1	TRP TRP	629	59.312	53.135	41.818	1.00 9.31	A	C
ATOM ATOM	4878	NE1	TRP	629 629	59. 635 60. 299	56.422	40.313	1.00 10.72	A	C
ATOM	4879		TRP	629	60. 779	55. 595 53. 126	39. 443 39. 379	1.00 10.74	A	N
ATOM	4880		TRP	629	59. 842	51.959	41. 295	1.00 12.40 1.00 11.95	A	C
ATOM	4881		TRP	629	60. 571	51.965	40.080	1.00 11.95	A A	C
ATOM	4882	C	TRP	629	58. 671	58. 722	42. 753	1.00 15.25	A	C C
ATOM	4883	ŏ	TRP	629	57. 622	59. 300	43. 012	1.00 15.58	A	Ö
ATOM	4884	Ň	SER	630	59.612	59. 269	41.983	1.00 16.99	A	N
ATOM	4885	CA	SER	630	59. 453	60.603	41.383	1.00 16.78	A	Č
ATOM	4886	CB	SER	630	58. 258	60.644	40. 421	1.00 18.65	A	Č
ATOM	4887	0G	SER	630	58. 531	59.987	39. 198	1.00 22.38	Ä	ŏ
ATOM	4888	Ċ	SER	630	59. 234	61.656	42. 450	1.00 16.69	Ä	č
ATOM	4889	0	SER	630	60.076	61.856	43. 321	1.00 17.90	. A	Ŏ,
ATOM	4890	N	TYR	631	58.093	62.335	42.368	1.00 17.21	A	N
ATOM	4891	CA	TYR	631	57. 737	63.362	43. 335	1.00 15.51	Ā	Ĉ
ATOM	4892	CB	TYR	631	56.380	63.969	42.981	1.00 17.16	Ä	Ċ
ATOM	4893	CG	TYR	631	56. 161	65.353	43.545	1.00 18.38	Ä	Č
ATOM	4894	CD1	TYR	631	55. 947	65.550	44.909	1.00 18.79	A	C
ATOM	4895		TYR	631	55. 741	66.826	45.429	1.00 19.48	Α	C C C
ATOM	4896	CD2		631	56.168	66.470	42.714	1.00 18.85	Α	C
ATOM	4897		TYR	631	55. 963	67.751	43. 226	1.00 19.30	Α	C
ATOM	4898	CZ	TYR	631	55. 748	67.918	44.580	1.00 19.21	Α	C
ATOM	4899	OH	TYR	631	55. 520	69. 173	45.084	1.00 20.71	Α	0

						FIG	. 4	- 101			(Continued)
ATOM 4901 0 TYR 631 57.946 63.201 45.731 1.00 13.23 A O ATOM 4902 N CLY 632 57.324 61.350 44.592 1.00 14.83 A N ATOM 4904 C CLY 632 58.653 60.477 46.394 1.00 14.83 A N ATOM 4905 0 CLY 632 58.653 60.477 46.394 1.00 14.53 A C ATOM 4906 N GLY 632 58.816 60.652 47.596 1.00 13.85 A O ATOM 4906 N GLY 633 61.030 60.185 46.014 1.00 14.69 A C ATOM 4908 C GLY 633 61.030 60.185 46.014 1.00 14.69 A C ATOM 4908 C GLY 633 61.050 61.513 46.576 1.00 15.25 A C ATOM 4908 D GLY 633 61.050 61.513 46.576 1.00 15.25 A C ATOM 4909 N TYR 634 61.058 62.598 45.994 1.00 13.67 A N ATOM 4910 N TYR 634 61.058 62.598 45.994 1.00 13.67 A N ATOM 4911 CA TYR 634 61.058 62.598 45.994 1.00 13.67 A N ATOM 4912 CD TYR 634 60.914 66.388 2.45.904 1.00 12.54 A C ATOM 4913 CG TYR 634 60.914 66.388 2.45.904 1.00 12.54 A C ATOM 4913 CG TYR 634 62.112 67.069 46.072 1.00 13.46 A C ATOM 4913 CG TYR 634 62.112 67.069 46.072 1.00 13.46 A C ATOM 4916 CD2 TYR 634 62.112 67.069 46.072 1.00 13.46 A C ATOM 4916 CD2 TYR 634 62.112 67.069 46.072 1.00 13.46 A C ATOM 4916 CD2 TYR 634 62.112 67.069 46.072 1.00 13.46 A C ATOM 4916 CD2 TYR 634 62.112 67.069 46.072 1.00 13.46 A C ATOM 4916 CD2 TYR 634 62.125 68.398 46.484 1.00 13.37 A C ATOM 4916 CD2 TYR 634 62.125 68.398 46.484 1.00 13.37 A C ATOM 4918 C TYR 634 60.957 70.375 47.091 1.00 12.54 A C ATOM 4918 C TYR 634 60.957 70.375 47.091 1.00 12.54 A C ATOM 4919 CC TYR 634 60.957 70.375 47.091 1.00 12.83 A C ATOM 4920 C TYR 634 60.957 70.375 47.091 1.00 12.83 A C ATOM 4920 C TYR 634 60.957 70.375 47.091 1.00 12.97 A O ATOM 4921 C TYR 634 60.957 70.375 47.091 1.00 12.97 A O A C ATOM 4920 C TYR 634 60.957 70.375 47.091 1.00 12.97 A O A C ATOM 4920 C TYR 634 60.957 70.975 68.383 60.984 60.985 1.00 12.97 A O A C ATOM 4920 C TYR 634 60.957 70.975 68.735 60.994 1.00 12.97 A O A C ATOM 4920 C TYR 634 60.957 70.975 68.735 60.00 12.977 A O A C ATOM 4920 C TYR 634 60.957 70.975 68.735 60.00 12.977 A O C ATOM 4930 C C TYR 634 60.958 60.958 60.00 12.90 10.00 19.90 A N A C ATOM 4920 C C TYR 634 60.958 60.958 60.00 10.00 19.90 A N A C				TYR	631					A	С
ATOM 4902 N GLY 632 57.324 61.350 44.592 1.00 14.83 A N A TOM 4904 C GLY 632 57.266 60.529 45.783 1.00 15.04 A C A TOM 4905 O GLY 632 58.653 60.477 46.394 1.00 14.53 A C A TOM 4906 N GLY 633 59.655 60.477 46.394 1.00 14.69 A C A TOM 4906 N GLY 633 61.030 60.185 46.014 1.00 14.69 A C A TOM 4907 CA GLY 633 61.030 60.185 46.014 1.00 14.69 A C A TOM 4909 O GLY 633 61.500 61.513 46.576 1.00 15.25 A C A TOM 4909 N GLY 633 61.500 61.513 46.576 1.00 15.25 A C A TOM 4909 N GLY 633 61.500 61.513 46.576 1.00 15.25 A C A TOM 4910 N TYR 634 61.058 62.598 45.954 1.00 13.29 A C A TOM 4911 CA TYR 634 61.418 63.940 46.398 1.00 13.29 A C A TOM 4912 CB TYR 634 60.914 66.382 45.904 1.00 12.54 A C A TOM 4914 CD TYR 634 62.112 67.069 46.954 45.397 1.00 11.67 A C A TOM 4916 CD TYR 634 62.112 67.069 46.094 45.397 1.00 11.67 A C A TOM 4916 CD TYR 634 62.112 67.069 46.094 45.001 13.37 A C A TOM 4916 CD TYR 634 62.125 68.398 46.484 1.00 13.37 A C A TOM 4917 CED TYR 634 62.125 68.398 46.484 1.00 13.37 A C A TOM 4916 CD TYR 634 60.933 69.049 46.734 1.00 12.53 A C A TOM 4917 CED TYR 634 60.933 69.049 46.734 1.00 12.33 A C A TOM 4917 CED TYR 634 60.933 69.049 46.734 1.00 12.33 A C A TOM 4910 OH TYR 634 60.957 70.375 47.091 1.00 12.83 A C A TOM 4910 OH TYR 634 60.957 70.375 47.091 1.00 12.83 A C A TOM 4920 V AL 635 59.486 60.957 70.375 47.091 1.00 12.97 A O A TOM 4920 V AL 635 59.486 60.957 70.375 47.091 1.00 12.97 A O A TOM 4921 OH TYR 634 60.957 70.375 47.091 1.00 12.97 A O A TOM 4922 N VAL 635 59.486 63.296 64.240 47.778 1.00 14.36 A C A C A TOM 4922 N VAL 635 59.486 63.296 64.240 47.778 1.00 14.36 A C A TOM 4922 N VAL 635 59.486 63.296 64.240 47.778 1.00 14.56 A C A TOM 4922 N VAL 635 59.486 63.296 64.240 47.778 1.00 14.56 A C A TOM 4930 CA THR 636 60.366 61.90 59.486 60.206 1.00 12.97 A O A TOM 4930 CA THR 636 60.607 60.386 61.098 50.855 1.00 18.40 A C A TOM 4930 CA THR 636 60.607 60.386 61.098 50.855 1.00 18.40 A C A TOM 4931 CB THR 636 60.607 60.386 61.098 50.855 1.00 18.40 A C A TOM 4931 CB THR 636 60.607 60.386 61.098 50.855 1.00 18.											
ATOM 4904 C GLY 632 55.663 60.529 45.783 1.00 15.04 A C ATOM 4905 0 GLY 632 58.816 60.552 47.596 1.00 13.85 A 0 ATOM 4906 N GLY 633 59.655 60.246 45.551 1.00 15.63 A N ATOM 4907 CA GLY 633 61.030 60.185 46.014 1.00 14.69 A C ATOM 4908 C GLY 633 61.500 61.513 46.576 1.00 15.25 A C ATOM 4908 C GLY 633 61.500 61.513 46.576 1.00 15.25 A C ATOM 4910 N TYR 634 61.058 62.251 61.561 47.555 1.00 16.82 A 0 ATOM 4910 N TYR 634 61.058 62.259 845.954 1.00 13.67 A N ATOM 4912 CB TYR 634 60.914 66.382 45.994 1.00 13.29 A C ATOM 4913 CG TYR 634 60.914 66.382 45.994 1.00 12.54 A C ATOM 4913 CG TYR 634 60.914 66.382 45.994 1.00 12.54 A C ATOM 4915 CE TYR 634 60.914 66.382 45.994 1.00 13.37 A C ATOM 4916 CD2 TYR 634 62.112 67.069 46.072 1.00 13.46 A C ATOM 4916 CD2 TYR 634 62.112 67.069 46.072 1.00 13.36 A C ATOM 4916 CD2 TYR 634 62.112 67.069 46.072 1.00 13.37 A C ATOM 4916 CD2 TYR 634 62.112 67.069 46.072 1.00 13.37 A C ATOM 4918 CZ TYR 634 60.914 66.382 45.994 1.00 12.54 A C ATOM 4916 CD2 TYR 634 60.933 69.049 46.734 1.00 12.54 A C ATOM 4916 CD2 TYR 634 60.933 69.049 46.734 1.00 12.57 A O A C ATOM 4918 CZ TYR 634 60.933 69.049 46.734 1.00 12.83 A C ATOM 4910 CT TYR 634 60.933 69.049 46.734 1.00 12.83 A C ATOM 4910 CT TYR 634 60.933 69.049 46.734 1.00 12.83 A C ATOM 4920 CT TYR 634 60.829 64.240 47.778 1.00 11.86 A C ATOM 4921 O TYR 634 60.829 64.240 47.778 1.00 12.87 A O A ATOM 4921 O TYR 634 60.829 64.240 47.778 1.00 12.83 A C ATOM 4921 O TYR 634 60.829 64.240 47.778 1.00 12.83 A C ATOM 4922 N VAL 635 59.542 63.968 47.949 1.00 16.82 A O A C ATOM 4924 CB VAL 635 59.542 63.968 47.949 1.00 14.36 A C A C ATOM 4924 CB VAL 635 59.596 61.60 61.60 61.628 A O A C ATOM 4924 CB VAL 635 59.50 69.64 63.71 1.00 12.00 12.00 A A C ATOM 4924 CB VAL 635 59.50 69.64 63.71 1.00 12.00 12.00 A A C ATOM 4930 CA THR 636 60.60 60.60 60.60 60.60 60.60 60.60 60.60 60.60 60.60 60.60 60.60 60.60 60.60 60.60 60.60 60.60 60.60 60.60 60.60 60.60 60.60 60.60 60.60 60.60 60.60 60.60 60.60 60.60 60.60 60.60 60.60 60.60 60.60 60.60 60.60 60.60 60.60 60.60 60.60						57. 324					
ATOM 4904 C GLY 632							60.529	45. 783			
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ATOM 4942 N MET 638 62.760 64.855 51.309 1.00 21.06 A N ATOM 4943 CA MET 638 62.490 66.074 52.066 1.00 21.87 A C ATOM 4944 CB MET 638 61.417 66.895 51.354 1.00 20.36 A C ATOM 4945 CG MET 638 61.876 67.465 50.032 1.00 21.23 A C ATOM 4946 SD MET 638 63.069 68.787 50.261 1.00 21.33 A S ATOM 4947 CE MET 638 62.006 70.229 50.125 1.00 19.31 A C										Α	
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ATOM 4945 CG MET 638 61.876 67.465 50.032 1.00 21.23 A C ATOM 4946 SD MET 638 63.069 68.787 50.261 1.00 21.33 A S ATOM 4947 CE MET 638 62.006 70.229 50.125 1.00 19.31 A C									_		C
ATOM 4946 SD MET 638 63.069 68.787 50.261 1.00 21.33 A S ATOM 4947 CE MET 638 62.006 70.229 50.125 1.00 19.31 A C											C
ATOM 4947 CE MET 638 62.006 70.229 50.125 1.00 19.31 A C											
ATOM 4040 C MPT 000 00 00 10. 20 00. 120 1. 00 13. 31 A	ATOM										
	ATOM										

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										(Continued)
					FI	G. 4	102			(00000000000000000000000000000000000000
ATOM	4949	0	MET	638	62.511	66. 351	54. 472	1.00 19.64	A	0
ATOM	4950	N	VAL	639	61.116			1.00 19.63	Ä	N
ATOM	4951	CA	VAL	639	60.611			1.00 20.04	Ā	C
ATOM	4952	CB	VAL	639	59. 524			1.00 20.08	Ā	C
ATOM	4953	CG1	VAL	639	59. 201			1.00 20.55	Ā	Ċ
ATOM	4954	CG2	VAL.	639	58. 275	63.879		1.00 17.95	A	C
ATOM	4955	C	VAL	639	61.758	63.793		1.00 20.25	Α	C
ATOM	4956	0	VAL	639	61.986	64. 185	56.831	1.00 23.11	Α	0
ATOM	4957	N	LEU	640	62.489	62.864	55.088	1.00 20.83	Α	N
ATOM	4958	CA	LEU	640	63.608	62. 225	55.765	1.00 22.08	Α	C
ATOM	4959	CB	LEU	640	64.245	61.179	54.855	1.00 22.31	Α	C
ATOM	4960	CG	LEU	640	63.400	59.939	54.570	1.00 21.31	Α	C
ATOM	4961		LEU	640	64. 143	59.041	53.611	1.00 22.16	Α	C
MOTA	4962		LEU	640	63. 105		55.863	1.00 22.25	A	C
ATOM	4963	C	LEU	640	64. 675		56.239	1.00 23.38	Α	C
ATOM	4964	0	LEU	640	65.416	62.922	57. 182	1.00 22.99	Α	0
ATOM	4965	N	GLY	641	64. 745		55. 592	1.00 23.16	Α	N
ATOM	4966	CA	GLY	641	65. 731	65.368	55. 972	1.00 23.10	Α	C
ATOM	4967	C	GLY	641	65. 153		56. 721	1.00 23.73	Α	C
ATOM	4968	0	GLY	641	65. 782	67.609	56.802	1.00 23.94	Α	0
ATOM	4969	N	SER	642	63. 958		57.278	1.00 22.74	Α	N
ATOM	4970	CA	SER	642	63. 318	67.484	58.002	1.00 20.76	Α	C
ATOM	4971	CB	SER	642	61. 798	67.370	57.883	1.00 19.77	Α	C
ATOM	4972	0G	SER	642	61. 319	66. 213	58.546	1.00 17.97	Α	0
ATOM	4973	C	SER	642	63. 723	67. 488	59.471	1.00 21.73	Α	C
ATOM	4974	0	SER	642	63. 656	68. 519	60.140	1.00 21.40	Α	0
ATOM	4975	N	GLY	643	64. 136	66. 327	59.967	1.00 22.24	Α	N
ATOM	4976	CA	GLY	643	64. 548	66. 213	61.350	1.00 22.64	Α	С
ATOM	4977	C	GLY	643	63. 407	65. 944	62.314	1.00 23.74	Α	С
ATOM	4978	0	GLY	643	63. 585	66.064	63. 528	1.00 25.32	A	0
ATOM	4979	N	SER	644	62. 244	65. 573	61.786	1.00 23.53	A	N
ATOM ATOM	4980	CA	SER	644	61.067	65. 301	62.616	1.00 23.38	A	C
ATOM	4981 4982	CB	SER	644	59.850	64. 995	61.742	1.00 24.79	A	C
ATOM	4983	OG C	SER	644	59. 898	63.666		1.00 24.45	A	0
ATOM	4984	0	SER SER	644	61.287	64. 129	63.559	1.00 23.18	A	C
ATOM	4985	N	GLY	644 645	60. 565	63.961	64.536	1.00 24.28	A	0
ATOM	4986	CA	GLY	645 645	62. 278	63.307	63. 258	1.00 23.27	A	N
ATOM	4987	C	GLY	645	62. 543	62. 166		1.00 24.80	A	C
ATOM	4988	0	GLY	645	61.398	61.175	64.114	1.00 24.80	A	C
ATOM	4989	N	VAL	646	61.379	60. 248	64. 920	1.00 27.93	A	0
ATOM	4990	CA	VAL	646	60. 446	61.357	63. 207	1.00 23.98	A	N
ATOM	4991	CB	VAL	646	59. 289 58. 092	60. 474 61. 207	63. 121	1.00 22.32	A	C
ATOM	4992	CG1		646	56. 945	60. 230	62. 473 62. 215	1.00 24.36	A	C
ATOM	4993	CG2		646	50. 945 57. 636	62. 351	63.381	1.00 22.37	A	C
ATOM	4994	C	VAL	646	59. 552	59. 202	62. 327	1.00 24.11	A	C
ATOM	4995	Õ	VAL	646	59. 079	59. 202 58. 128	62. 690	1.00 21.28 1.00 21.25	A	C
ATOM	4996	N	PHE	647	60. 303	59. 326	61. 239	1.00 21.25	A	0 N
ATOM	4997	CA	PHE	647	60. 593	58. 182	60. 380	1.00 21.00	A A	N C
		V. 1		0.11	00,000	00. I UL	30.000	1.00 10.00	Л	U

					FI	G. 4	- 103			(Continued)	I
ATOM ATOM	4998 4999	CB CG	PHE PHE	647 647	60. 497 59. 142	7 58.615	58. 924		A A	C C	
ATOM	5000	CD1	PHE	647	58.138	58.258	58. 152	1.00 15.39	Α	С	
ATOM ATOM	5001 5002		PHE	647 647	58. 841 56. 858				A A	C C	
ATOM	5003	CE2	PHE	647	57. 562	60.943	58. 423		A	С	
ATOM ATOM	5004 5005	CZ C	PHE PHE	647 647	56. 568	60.061	58. 031	1.00 13.75	A	C	
ATOM	5006	Õ	PHE	647	61. 944 62. 943			1.00 18.46 1.00 20.84	A A	C 0	
ATOM	5007	N	LYS	648	61.958	56.232	60.722	1.00 17.11	A	Ň	
ATOM ATOM	5008 5009	CA CB	LYS	648	63. 165			1.00 19.06	A	C	
ATOM	5010	CG	LYS LYS	648 648	62. 789 63. 961		61.545 61.955	1.00 17.86 1.00 17.94	A A	C C	
ATOM	5011	CD	LYS	648	63. 484		62. 405	1.00 17.54	A	C	
ATOM	5012	CE	LYS	648	64. 594			1.00 19.22	Α	C	
ATOM ATOM	5013 5014	NZ C	LYS LYS	648 648	65. 757 64. 025		62. 204 59. 747	1.00 20.59 1.00 21.47	A A	N C	
ATOM	5015	ŏ	LYS	648	65. 251		59. 815	1.00 21.47	A	0	
ATOM	5016	N	CYS	649	63. 376	55.094	58.610	1.00 22.38	Α	N	
ATOM ATOM	5017 5018	CA C	CYS CYS	649 649	64. 077 63. 156		57. 353	1.00 24.23	A	C	
ATOM	5019	Õ	CYS	649	61.939		56. 181 56. 342	1.00 24.09 1.00 23.94	A A	C 0	
ATOM	5020	CB	CYS	649	64.527	53.447	57. 237	1.00 27.68	A	č	
ATOM ATOM	5021 5022	SG N	CYS GLY	649	63. 130		57. 313	1.00 32.05	A	S	
ATOM	5022	CA	GLY	650 650	63. 746 62. 961	55. 426 55. 757	55. 004 53. 834	1.00 21.50 1.00 21.04	A A	N C	
ATOM	5024	C	GLY	650	63. 649	55. 384	52. 535	1.00 21.13	A	C	
ATOM	5025	0	GLY	650	64. 874	55. 333	52.474	1.00 21.62	, A	0	
ATOM ATOM	5026 5027	N CA	ILE ILE	651 651	62. 857 63. 388	55. 124 54. 753	51. 499 50. 195	1.00 19.35	A	N	
ATOM	5028	CB	ILE	651	62. 896	53. 352	49. 758	1.00 19.18 1.00 19.03	A A	C C	
ATOM	5029		ILE	651	63.601	52.933	48. 481	1.00 17.31	Ä	č	
ATOM ATOM	5030 5031	CG1 CD1	ILE	651	63. 173	52. 326	50. 853	1.00 19.60	A	C	
ATOM	5032	CDI	ILE	651 651	62. 827 62. 953	50. 901 55. 749	50. 456 49. 120	1.00 18.48 1.00 19.53	A A	C	
ATOM	5033	0	ILE	651	61.758	56.015	48. 949	1.00 19.77	A A	C 0	
ATOM	5034		ALA	652	63.925	56. 292	48. 393	1.00 18.34	Α	N	
ATOM ATOM	5035 5036		ALA ALA	652 652	63. 633 64. 323	57. 240 58. 574	47.324	1.00 15.69	A	C	
ATOM	5037		ALA	652	64. 107	56.662	47. 594 45. 996	1.00 14.05 1.00 14.98	A A	C C	
ATOM	5038	0	ALA	652	65. 288	56. 367	45. 827	1.00 14.12	Ä	ŏ	
ATOM ATOM	5039		VAL	653	63. 175	56. 487	45.064	1.00 14.68	A	N	
ATOM	5040 5041		VAL VAL	653 653	63. 492 62. 582	55. 963 54. 754	43. 738 43. 366	1.00 14.84 1.00 17.41	A A	C C	
ATOM	5042	CG1	VAL	653	62. 865	54. 291	41.932	1.00 17.41	A	C .	
ATOM	5043	CG2		653	62. 806	53.607	44.352	1.00 18.10	Α	C	
ATOM ATOM	5044 5045		VAL VAL	653 653	63. 292 62. 224	57. 063 57. 660	42.694	1.00 13.22	A	C	
ATOM			ALA	654	64. 331	57. 669 57. 317	42.620 41.901	1.00 11.12 1.00 12.68	A A	O N	
						= -				••	

					FIG. 4-104	(Continued)
ATOM ATOM ATOM	5047 5048 5049	CB	ALA ALA ALA		64. 289 58. 327 40. 845 1. 00 10. 68 A 63. 513 57. 790 39. 650 1. 00 7. 27 A	C C
ATOM ATOM	5050 5051	0 (ALA PRO	654 655	63. 653 59. 607 41. 352 1. 00 10. 02 A 62. 687 60. 103 40. 787 1. 00 13. 18 A 64. 208 60. 179 42. 420 1. 00 10. 68 A	C 0
ATOM ATOM	5052 5053	CD	PRO PRO	655 655	65. 319 59. 696 43. 262 1. 00 8. 01 A	N C
ATOM ATOM	5054 5055	CB	PRO PRO	655 655	64. 092 61. 344 44. 422 1. 00 8. 50 A	C C
ATOM ATOM	5056 5057	C	PRO PRO	655 655	64. 090 62. 714 42. 327 1. 00 12. 92 A	C C
ATOM ATOM	5058 5059	N	VAL VAL	656 656	63. 245 63. 735 42. 454 1. 00 12. 39 A 63. 612 65. 065 41. 999 1. 00 12. 85 A	O N C
ATOM ATOM	5060 5061		VAL VAL	656 656	62. 373 65. 946 41. 769 1. 00 11. 42 A 62. 781 67. 416 41. 645 1. 00 10. 52 A	C C
ATOM ATOM	5062 5063	C	VAL VAL	656 656	61. 661 65. 500 40. 510 1. 00 10. 18 A 64. 382 65. 560 43. 236 1. 00 13. 79 A	C C
ATOM ATOM ATOM	5064 5065 5066	N	VAL SER	656 657	64. 038 65. 188 44. 355 1. 00 14. 63 A 65. 419 66. 372 43. 066 1. 00 14. 27 A	O N
ATOM ATOM	5067 5068	CA CB OG	SER SER SER	657 657 657	66. 174 66. 831 44. 238 1. 00 14. 99 A 67. 589 66. 231 44. 231 1. 00 15. 67 A 68. 385 66. 819 43. 213 1. 00 15. 19 A	C C
ATOM ATOM	5069 5070	C 0	SER SER	657 657	68. 385 66. 819 43. 213 1. 00 15. 19 A 66. 286 68. 343 44. 320 1. 00 14. 77 A 66. 387 68. 912 45. 406 1. 00 14. 39 A	0 C 0
ATOM ATOM	5071 5072	N CA	ARG ARG	658 658	66. 269 68. 978 43. 158 1. 00 15. 05 A 66. 388 70. 423 43. 038 1. 00 16. 33 A	N C
ATOM ATOM	5073 5074	CB CG	ARG ARG	658 658	67. 845 70. 787 42. 747 1. 00 20. 44 A 68. 142 72. 274 42. 582 1. 00 24. 34 A	C C
ATOM ATOM ATOM	5075 5076 5077	CD NE CZ	ARG ARG ARG	658 658 658	69. 543 72. 450 42. 025 1. 00 25. 38 A 69. 905 73. 838 41. 757 1. 00 25. 70 A	C N
ATOM ATOM	5078 5079	NH1	ARG ARG	658 658	70. 353 74. 683 42. 676 1. 00 28. 34 A 70. 491 74. 288 43. 935 1. 00 28. 23 A 70. 690 75. 916 42. 329 1. 00 29. 55 A	C N
ATOM ATOM	5080 5081	C O	ARG ARG	658 658	70. 690 75. 916 42. 329 1. 00 29. 55 A 65. 515 70. 775 41. 850 1. 00 15. 87 A 65. 752 70. 288 40. 735 1. 00 16. 75 A	N C O
ATOM ATOM	5082 5083	N CA	TRP TRP	659 659	64.514 71.616 42.073 1.00 13.52 A 63.603 71.967 40.999 1.00 13.69 A	N C
ATOM ATOM ATOM	5084 5085		TRP TRP	659 659	62. 465 72. 823 41. 550 1. 00 13. 63 A 61. 504 71. 963 42. 341 1. 00 17. 48 A	Č C
ATOM ATOM ATOM	5086 5087 5088	CD2 CE2 CE3	TRP	659 659 659	60. 690 70. 898 41. 829 1. 00 16. 63 A 60. 027 70. 313 42. 927 1. 00 18. 08 A 60. 460 70. 382 40. 547 1. 00 16. 21 A	C C
ATOM ATOM	5089 5090	CD1 NE1	TRP	659 659	60. 460 70. 382 40. 547 1. 00 16. 21 A 61. 300 71. 980 43. 692 1. 00 17. 21 A 60. 418 70. 993 44. 050 1. 00 17. 37 A	C C N
ATOM ATOM	5091 5092	CZ2 CZ3	TRP TRP	659 659	59. 145 69. 233 42. 785 1. 00 21. 55 A 59. 584 69. 311 40. 403 1. 00 18. 00 A	N C C
ATOM ATOM	5093 5094		TRP	659 659	58. 937 68. 746 41. 516 1. 00 20. 15 A 64. 219 72. 580 39. 748 1. 00 13. 15 A	C C
ATOM	5095	0	TRP	659	63.643 72.503 38.670 1.00 11.17 A	0

		FIG. 4-105	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	5096 N GLU 66 5097 CA GLU 66 5098 CB GLU 66 5099 CG GLU 66 5100 CD GLU 66 5101 OE1 GLU 66 5102 OE2 GLU 66 5103 C GLU 66 5104 O GLU 66 5105 N TYR 66 5106 CA TYR 66 5107 CB TYR 66 5108 CG TYR 66	65. 400 73. 163 39. 871 1. 00 14. 12 66. 042 73. 725 38. 697 1. 00 15. 96 67. 147 74. 704 39. 108 1. 00 16. 83 66. 548 76. 001 39. 626 1. 00 19. 65 67. 535 76. 901 40. 313 1. 00 22. 71 68. 310 77. 600 39. 617 1. 00 25. 18 67. 527 76. 907 41. 561 1. 00 23. 59 66. 577 72. 635 37. 777 1. 00 15. 29 67. 001 72. 922 36. 659 1. 00 16. 67 1 66. 539 71. 383 38. 233 1. 00 14. 54 67. 003 70. 269 37. 399 1. 00 14. 57 1 67. 642 69. 154 38. 230 1. 00 13. 59 1 68. 878 69. 504 39. 035 1. 00 15. 73	A N A C A C A O A C A C A C A C A C A C A C
ATOM ATOM ATOM ATOM	5109 CD1 TYR 66 5110 CE1 TYR 66 5111 CD2 TYR 66 5112 CE2 TYR 66 5113 CZ TYR 66	70. 889 70. 805 39. 390 1. 00 12. 74 69. 199 68. 765 40. 166 1. 00 16. 63 70. 338 69. 027 40. 898 1. 00 16. 03 71. 183 70. 041 40. 515 1. 00 13. 47	A C A C A C A C A C A C A C
ATOM ATOM ATOM ATOM ATOM ATOM	5114 OH TYR 661 5115 C TYR 661 5116 O TYR 661 5117 N TYR 662 5118 CA TYR 662 5119 CB TYR 662	65. 842 69. 637 36. 608 1. 00 15. 74 66. 077 68. 854 35. 675 1. 00 13. 97 64. 602 69. 963 36. 984 1. 00 13. 28 63. 445 69. 390 36. 308 1. 00 13. 00	A 0 A C A 0 A N A C
ATOM ATOM ATOM ATOM ATOM	5120 CG TYR 662 5121 CD1 TYR 662 5122 CE1 TYR 662 5123 CD2 TYR 662 5124 CE2 TYR 662	61. 395 68. 026 36. 862 1. 00 14. 50 60. 010 68. 199 36. 802 1. 00 15. 74 59. 184 67. 201 36. 273 1. 00 14. 99 61. 930 66. 825 36. 400 1. 00 14. 83	A C A C A C A C A C
ATOM ATOM ATOM ATOM ATOM	5125 CZ TYR 662 5126 OH TYR 662 5127 C TYR 662 5128 O TYR 662 5129 N ASP 663	59. 756 66. 024 35. 804 1. 00 15. 11 58. 983 65. 060 35. 214 1. 00 17. 05 62. 964 70. 251 35. 135 1. 00 12. 46 63. 320 71. 423 35. 030 1. 00 12. 22 62. 147 69. 673 34. 260 1. 00 12. 09	A C A C A O A C A O A N
ATOM ATOM ATOM ATOM ATOM ATOM	5130 CA ASP 663 5131 CB ASP 663 5132 CG ASP 663 5133 OD1 ASP 663 5134 OD2 ASP 663 5135 C ASP 663	61. 686 70. 394 33. 076 1. 00 13. 20 60. 998 69. 427 32. 099 1. 00 11. 88 59. 668 68. 925 32. 606 1. 00 13. 51 59. 476 67. 692 32. 633 1. 00 14. 06 58. 809 69. 758 32. 962 1. 00 11. 87	A C A C A C A O A O
ATOM ATOM ATOM ATOM ATOM	5135 C ASP 663 5136 O ASP 663 5137 N SER 664 5138 CA SER 664 5139 CB SER 664 5140 OG SER 664	60. 807 71. 625 33. 300 1. 00 13. 03 60. 036 71. 713 34. 260 1. 00 12. 71 60. 945 72. 576 32. 383 1. 00 12. 83 60. 210 73. 829 32. 425 1. 00 13. 80 60. 433 74. 600 31. 120 1. 00 14. 92 59. 996 73. 851 30. 000 1. 00 14. 78	A C A O A N A C A C
ATOM ATOM ATOM ATOM	5141 C SER 664 5142 O SER 664 5143 N VAL 665 5144 CA VAL 665	59. 996 73. 851 30. 000 1. 00 14. 78 58. 715 73. 688 32. 674 1. 00 13. 35 58. 234 73. 974 33. 762 1. 00 15. 82 57. 987 73. 247 31. 658 1. 00 13. 43 56. 540 73. 101 31. 733 1. 00 14. 34	A O A C A O A N A C

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				(Continued)
			FIG. 4-106	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	5146 CG1 V 5147 CG2 V 5148 C V 5149 O V 5150 N T 5151 CA T 5152 CB T 5153 CG T 5154 CD1 T 5155 CE1 T 5156 CD2 T 5157 CE2 T 5158 CZ T 5158 CZ T 5159 OH T 5160 C T 5161 O T 5162 N TI 5163 CA TI 5164 CB TI	AL 665 AL 665 AL 665 YR 666 YR 667 IR 667 IR 667	FIG. 4 - 106 56.027 72.182 30.602 1.00 14.98 A 54.496 72.131 30.615 1.00 15.10 A 56.537 72.690 29.263 1.00 13.19 A 55.972 72.620 33.070 1.00 14.50 A 55.153 73.302 33.677 1.00 14.33 A 56.392 71.452 33.534 1.00 15.45 A 55.876 70.948 34.801 1.00 17.06 A 56.323 69.501 35.038 1.00 15.58 A 55.839 68.903 36.349 1.00 15.58 A 55.839 68.903 36.349 1.00 13.94 A 54.692 68.119 36.395 1.00 14.70 A 54.276 67.517 37.577 1.00 13.28 A 56.560 69.080 37.534 1.00 13.77 A 56.154 68.482 38.727 1.00 13.27 A 55.012 67.700 38.737 1.00 12.27 A 55.012 67.700 38.737 1.00 12.27 A 55.012 67.700 38.737 1.00 15.52 A 54.609 67.072 39.896 1.00 18.37 A 56.297 71.796 35.998 1.00 17.89 A 55.451 72.200 36.795 1.00 19.29 A 57.592 72.066 36.125 1.00 17.90 A 58.092 72.833 37.265 1.00 19.74 A 59.621 72.953 37.251 1.00 18.84	(Continued) C C C C C C C C C C C C C C C C C C
ATOM ATOM	5165 OG1 TI 5166 CG2 TI	IR 667 IR 667	60. 206 71. 675 36. 968 1. 00 20. 18 A 60. 108 73. 441 38. 604 1. 00 17. 74 A	C O C
ATOM ATOM ATOM	5168 O TF 5169 N GI	.U 668	57. 537 74. 246 37. 339 1. 00 21. 44 A 56. 916 74. 635 38. 333 1. 00 21. 51 A 57. 778 75. 011 36. 280 1. 00 21. 85 A	C O N
ATOM ATOM ATOM	5170 CA GI 5171 CB GI 5172 CG GI	U 668	57. 330 76. 389 36. 200 1. 00 21. 18 A 57. 746 76. 976 34. 859 1. 00 20. 69 A 59. 251 77. 096 34. 703 1. 00 20. 20 A	C C C
ATOM ATOM ATOM	5173 CD GL 5174 OE1 GL 5175 OE2 GL	U 668	59. 657 77. 559 33. 322 1. 00 19. 55 A 58. 783 78. 068 32. 588 1. 00 19. 49 A	C 0
ATOM ATOM ATOM	5176 C GL 5177 O GL 5178 N AR	U 668 U 668	55. 828 76. 517 36. 394 1. 00 21. 50 A 55. 339 77. 559 36. 814 1. 00 22. 31 A	0 C 0
ATOM ATOM	5179 CA AR 5180 CB AR	G 669 G 669	55. 098 75. 449 36. 101 1. 00 21. 90 A 53. 648 75. 458 36. 249 1. 00 21. 18 A 53. 060 74. 121 35. 786 1. 00 22. 06 A	N C C
ATOM ATOM ATOM	5181 CG AR 5182 CD AR 5183 NE AR	G 669	51. 546 74. 026 35. 922 1. 00 21. 37 A 51. 085 72. 625 35. 653 1. 00 20. 85 A	C
ATOM ATOM	5184 CZ AR 5185 NH1 AR	G 669 G 669	51. 667 70. 918 33. 981 1. 00 21. 10 A 51. 522 69. 962 34. 888 1. 00 19. 62 A	N C N
ATOM ATOM ATOM	5186 NH2 ARG 5187 C ARG 5188 O ARG	G 669	52. 018 70. 610 32. 741 1. 00 20. 23 A 53. 246 75. 706 37. 695 1. 00 21. 23 A	N C
ATOM ATOM ATOM	5189 N TYI 5190 CA TYI	R 670 R 670	54. 067 75. 239 38. 631 1. 00 21. 65 A 53. 771 75. 409 40. 047 1. 00 22. 27 A	O N C
ATOM ATOM	5191 CB TYI 5192 CG TYI 5193 CD1 TYI	R 670	53. 113 72. 930 39. 972 1. 00 20. 47 A	C C C
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ATOM	5194	CE1		670	53. 321	70.985	38.537	1.00 22.18	A	C
ATOM	5195	CD2		670	51.726	72.831	39.850	1.00 19.78	A	C
ATOM	5196	CE2	TYR	670	51.139	71.831	39.079	1.00 19.87	Α	C
ATOM	5197	CZ	TYR	670	51.944	70.911	38. 422	1.00 22.17	Ā	Ċ
ATOM	5198	OH	TYR	670	51.388	69. 931	37. 623	1.00 23.11	A	ŏ
ATOM	5199	C	TYR	670	54. 769	76.317	40. 757	1.00 23.11		C
									A	
ATOM	5200	0	TYR	670	54. 442	76.937	41.763	1.00 24.86	A	0
ATOM	5201	N	MET	671	55. 983	76.404	40. 228	1.00 24.66	A	N
ATOM	5202	CA	MET	671	57.029	77.207	40.851	1.00 23.96	A	C
ATOM	5203	CB	MET	671	58. 327	76.400	40.905	1.00 24.00	A	C
ATOM	5204	CG	MET	671	58. 288	75.215	41.852	1.00 23.55	A	C
ATOM	5205	SD	MET	671	58. 383	75.732	43.565	1.00 24.97	Α	S
ATOM	5206	CE	MET	671	60.159	75.998	43.721	1.00 21.94	Α	C
ATOM	5207	C	MET	671	57.330	78.547	40. 203	1.00 24.00	A	Č
ATOM	5208	Ŏ	MET	671	58. 101	79. 331	40.756	1.00 25.98	Ä	ŏ
ATOM	5209	Ň	GLY	$67\hat{2}$	56. 741	78. 822	39.045	1.00 22.07	A	N
ATOM	5210	CA	GLY	672	57.044	80.076	38. 379	1.00 22.07		
ATOM	5211	C	GLY	672					A	C
					58.472	80.028	37. 857	1.00 22.69	A	C
ATOM	5212	0	GLY	672	59.005	78. 947	37.641	1.00 23.27	A	0
ATOM	5213	N	LEU	673	59. 108	81.180	37.667	1.00 22.65	A	N
ATOM	5214	CA	LEU	673	60.477	81. 209	37. 151	1.00 20.90	A	С
ATOM	5215	CB	LEU	673	60.626	82.356	36.164	1.00 19.50	A	C
ATOM	5216	CG	LEU	673	59.639	82. 282	35.010	1.00 19.96	A	C
ATOM	5217		LEU	673	59.779	83.513	34.147	1.00 20.87	Α	С
ATOM	5218	CD2	LEU	673	59.892	81.027	34.203	1.00 21.63	Α	C
ATOM	5219	C	LEU	673	61.528	81.344	38. 248	1.00 21.08	A	C
ATOM	5220	0	LEU	673	61.313	82.028	39.239	1.00 21.87	Ä	Ö
ATOM	5221	N	PRO	674	62.692	80.700	38.072	1.00 21.90	Ä	Ň
ATOM	5222	CD	PRO	674	63.050	79. 803	36.968	1.00 21.16	Ä	C
ATOM	5223	CA	PRO	674	63.780	80. 747	39.050	1.00 23.23	A	Č
ATOM	5224	CB	PRO	674	64.618	79.510	38. 709	1.00 21.90	A	Č
ATOM	5225	CG	PRO	674	63. 803	78. 755	37. 695	1.00 21.30		Č
ATOM	5226	C	PRO	674	64.617	82. 023	38.943	1.00 24.90	A	
ATOM	5227	Ö	PRO	674	65. 841	81.977			A	C
ATOM	5228	N	THR	675	63.966		39. 028		A	0
ATOM	5229	CA	THR	675		83. 158	38. 743	1.00 25.88	Ą	N
ATOM	5230				64.695	84. 411	38. 640	1.00 27.60	A	C
		CB	THR	675	64. 208	85. 237	37. 447	1.00 27.12	Ą	C
ATOM	5231	0G1		675	62.811	85. 524	37. 599	1.00 29.30	A	0
ATOM	5232		THR	675	64. 431	84. 471	36. 156	1.00 25.59	A	C
ATOM	5233	C	THR	675	64. 496	85. 211	39.918	1.00 28.74	A	C
ATOM	5234	0	THR	675	63. 543	84. 982	40.660	1.00 29.47	A	0
ATOM	5235		PRO	676	65. 404	86. 156	40. 200	1.00 ·29.41	A	N
ATOM	5236		PRO	676	66.625	86.508	39. 457	1.00 28.96	Α	С
ATOM	5237		PRO	676	65. 284	86.969	41.411	1.00 29.70	Α	C
ATOM	5238		PRO	676	66.465	87.929	41.299	1.00 28.87	Α	C
ATOM	5239	CG	PRO	676	67.467	87.142	40.533	1.00 28.27	Α	Č
ATOM	5240	C	PRO	676	63.948	87.707	41.484	1.00 30.03	Ä	Č
ATOM	5241	0	PRO	676	63.359	87.829	42.558	1.00 29.93	Ä	ŏ
ATOM	5242	N	GLU	677	63.463	88. 190	40.343	1.00 30.62	Ä	Ň
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ATOM	5243	CA	GLU	677	62. 203	22	. 923	40.348	1.00 3	ก ๑๑	Α	C	
ATOM	5244	CB	GLU	677	62. 192		. 013	39. 264	1.00 3		A	C	
ATOM	5245	CG	GLU	677	62. 103		. 536	37. 821	1.00 3		A		
ATOM	5246	CD	GLU	677	63. 380		. 877	37. 331	1.00 3		A	C C	
ATOM	5247		GLU	677	64. 480		. 356	37. 697	1.00 3		A	Õ	
ATOM	5248		GLU	677	63. 276		. 891	36.566	1.00 3		A	0	
ATOM	5249	C	GLU	677	60. 952		. 065	40. 231	1.00 3		A	Č	
ATOM	5250	0	GLU	677	59. 893		. 564	39. 849	1.00 3		A	0	
ATOM	5251	N	ASP	678	61.067		. 304 . 777	40. 546	1.00 3		A	N	
ATOM	5252	CA	ASP	678	59.906		. 897	40. 523	1.00 20		A	C	
ATOM	5253	CB	ASP	678	59. 833		. 048	39. 253	1.00 2				
ATOM	5254	CG	ASP	678	58. 472		. 359	39. 097	1.00 2		A	C	
ATOM	5255		ASP	678	57. 885		. 980	40. 128	1.00 2		A	0 0	
ATOM	5256		ASP	678	57. 980		. 380 . 189	37. 956	1.00 28		A		
ATOM	5257	C	ASP	678	59. 920		. 169 . 982	41.737			A	0	
ATOM	5258	0	ASP	678	59. 481		. 382	42.810	1.00 25 1.00 25		A	C	
ATOM	5259	N	ASN	679	60. 442		. 768	41.591			A	0 N	
ATOM	5260	CA	ASN	679	60. 442		. 835	42. 708	1.00 23		A	N	
ATOM	5261	CB	ASN	679	59. 326			42. 108	1.00 21 1.00 19		A	C	
ATOM	5262	CG	ASN	679	58. 894		. 818 . 146	42. 490	1.00 19		A	C	
ATOM	5263		ASN	679	58. 491		. 140 . 981	43. 775	1.00 1:		A	C	
ATOM	5264		ASN	679	58. 957		. 879	44. 882	1.00 20		A	<i>N</i> i	
ATOM	5265	C	ASN	679	61. 760		. 099	42. 957	1.00 13		A	N	
ATOM	5266	Õ	ASN	679	61.770		. 055	43. 601	1.00 21		A A	C 0	
ATOM	5267	N	LEU	680	62. 873		. 636	42. 472	1.00 24			N.	
ATOM	5268	CA	LEU	680	64. 164		. 967	42. 665	1.00 26		A A	C	
ATOM	5269	CB	LEU	680	65. 316		. 842	42. 157	1.00 26				
ATOM	5270	CG	LEU	680	66. 726		. 275	42. 385	1.00 28		A A	C C	
ATOM	5271		LEU	680	66. 844		903	41.747	1.00 20		A	C	
ATOM	5272		LEU	680	67. 772		211	41.801	1.00 29		A	Č	
ATOM	5273	C	LEU	680	64. 449		556	44. 109	1.00 23		A	Č	
ATOM	5274	ŏ	LEU	680	64. 977		471	44. 347	1.00 28		A	0	
ATOM	5275	N	ASP	681	64. 111		411	45. 072	1.00 27		A	N	
ATOM	5276	CA	ASP	681	64. 360		091	46. 475	1.00 28		A	C	
ATOM	5277	CB	ASP	681	63. 836		196	47. 394	1.00 30		A	Č	
ATOM	5278	CG	ASP	681	64. 774		386	47. 473	1.00 34		A	Č	
ATOM	5279		ASP	681	65. 908		289	46. 952	1.00 35		A	Õ	
ATOM	5280		ASP	681	64.380		417	48.067	1.00 36		A	Ö	
ATOM	5281	C	ASP	681	63. 773		753	46. 920	1.00 27		A	Č	
ATOM	5282	Ŏ	ASP	681	64. 428		005	47.647	1.00 28		A	Õ	
ATOM	5283	Ň	HIS	682	62. 551		438	46. 502	1.00 25		A	N	
ATOM	5284	CA	HIS	682	61.981		164	46.913	1.00 25		A	Č	
ATOM	5285	CB	HIS	682	60. 456		161	46.801	1.00 25		Ä	Č	
ATOM	5286	ĊĞ	HIS	682	59. 832		914	47. 349	1.00 27		A	Č	
ATOM	5287		HIS	682	59. 091		948	46. 754	1.00 27		A	Č	
ATOM	5288		HIS	682	60. 021		503	48.650	1.00 26		Ä	N	
ATOM	5289		HIS	682	59. 428		336	48. 832	1.00 26		Ä	C	
ATOM	5290		HIS	682	58. 857		977	47. 697	1.00 25		A	N	
ATOM	5291	C	HIS	682	62.559		983	46. 130	1.00 24		A	Ċ	

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ATOM	5292		HIS	682	62. 463	76. 837		1.00 23.47	Α	0
ATOM ATOM	5293 5294		TYR TYR	683	63. 144	78. 258		1.00 23.49	A	N
ATOM	5295	CB	TYR	683 683	63. 768 64. 249	77. 208 77. 758		1.00 22.64	A	C
ATOM	5296	CG		683	63. 291	77. 594		1.00 20.68 1.00 19.28	A A	C C C C
ATOM	5297		TYR	683	63. 325	76. 461	40.857	1.00 15.28	A	Č
ATOM	5298	CE	TYR	683	62. 464	76. 317	39. 783	1.00 16.23	A	Č
ATOM	5299		2 TYR	683	62.361	78. 589	41.347	1.00 20.47	A	č
ATOM	5300		2 TYR	683	61.495	78. 453	40.276	1.00 20.17	Ā	Č
ATOM	5301	CZ	TYR	683	61.554	77. 314		1.00 19.09	Α	C
ATOM	5302	OH	TYR	683	60. 695	77. 176	38. 441	1.00 21.54	Α	0
ATOM	5303	C	TYR	683	64. 989	76. 727	44. 924	1.00 22.32	A	C
ATOM ATOM	5304 5305	0 N	TYR	683	65. 189	75. 533	45. 125	1.00 22.65	A	0
ATOM	5306	CA	ARG ARG	684 684	65. 799 67. 025	77. 685 77. 392	45.355	1.00 22.44	A	N
ATOM	5307	CB	ARG	684	67. 928	78. 624	46. 076 46. 071	1.00 22.97 1.00 22.89	A	C
ATOM	5308	CG	ARG	684	68. 349	79.064	44. 672	1.00 24.89	A A	C C
ATOM	5309	CD	ARG	684	69. 238	78. 020	44.004	1.00 24.31	A	C
ATOM	5310	NE	ARG	684	69. 328	78. 223	42.562	1.00 25.47	A	N
ATOM	5311	CZ	ARG	684	69.844	79. 299	41.974	1.00 27.89	Ä	Ç .
ATOM	5312		ARG	684	70. 337	80. 294	42.703	1.00 29.09	Ä	Ň
ATOM	5313		ARG	684	69.846	79. 388	40.648	1.00 27.04	Α	N
ATOM	5314	C	ARG	684	66.807	76. 922	47. 501	1.00 22.90	Α	С
ATOM	5315	0	ARG	684	67. 711	76.368	48.111	1.00 24.16	Α	0
ATOM ATOM	5316	N	ASN	685	65.608	77. 121	48.030	1.00 24.64	A	N
ATOM	5317 5318	CA CB	ASN ASN	685 685	65. 331	76. 715	49.399	1.00 24.41	A	C
ATOM	5319	CG	ASN	685 685	64. 599	77. 831	50.134	1.00 28.42	A	C
ATOM	5320		ASN	685	64. 455 65. 410	77. 547 77. 117	51.610 52.266	1.00 34.24	A	C
ATOM	5321		ASN	685	63. 264	77. 791	52. 200 52. 150	1.00 38.25 1.00 37.49	. A A	0
ATOM	5322	C	ASN	685	64. 545	75. 419	49. 537	1.00 37.43	A	N C
ATOM	5323	0	ASN	685	64. 356	74. 929	50.649	1.00 23.86	A	0
ATOM	5324	N	SER	686	64. 101	74.852	48.417	1.00 21.55	A	Ň
ATOM	5325	CA	SER	686	63.336	73.613		1.00 19.71	Ä	Ĉ
ATOM	5326	CB	SER	686	61.976	73.811	47.774	1.00 19.20	Α	Č
ATOM	5327	0G	SER	686	62.114	74.112	46.397	1.00 15.00	Α	0
ATOM	5328	C	SER	686	64.060	72. 421	47.823	1.00 20.13	Α	C
ATOM ATOM	5329	0 N	SER	686	63. 447	71.611	47.128	1.00 21.27	A	0
ATOM	5330 5331	N CA	THR THR	687 687	65. 362	72. 307	48.060	1.00 19.02	A	N
ATOM	5332	CB	THR	687	66. 122 67. 441	71.189	47.509	1.00 17.15	A	C
ATOM	5333	OG1	THR	687	68. 362	71.665 71.959	46. 906 47. 960	1.00 16.10	A	C
ATOM	5334		THR	687	67. 214	72. 920	46.058	1.00 17.42 1.00 14.71	A A	0 C
ATOM	5335	C	THR	687	66. 433	70. 153	48. 585	1.00 14.71	A	C
ATOM	5336	0	THR	687	66. 496	70.466	49. 763	1.00 15.82	A	Ö
ATOM	5337	N	VAL	688	66. 627	68. 908	48. 182	1.00 18.43	Ä	N
ATOM	5338	CA	VAL	688	66. 935	67.854	49.147	1.00 17.92	Ä	Č
ATOM	5339	CB	VAL	688	66.840	66. 453	48.480	1.00 17.13	Ā	Č
ATOM	5340	CG1	VAL	688	67.092	65. 352	49.503	1.00 15.01	Α	С

					FI	G. 4	-110)		(Continued)
ATOM	5341		2 VAL		65. 459	66.279	47.845	1.00 18.49	A	C .
ATOM	5342		VAL		68. 341	68.059			Ā	Č
ATOM	5343		VAL		68. 559	67.905	50.923		Ā	0
ATOM	5344		MET		69. 280	68.428	48.851		A	N
ATOM	5345				70. 672	68.647	49.246		A	C
ATOM	5346	CB	MET		71.475		48.065		A	Č
ATOM	5347	CG	MET		71.829		46.984		Α	Ċ
ATOM	5348		MET		70. 465		45.909	1.00 11.73	Α	S
ATOM	5349	CE	MET	689	70. 338			1.00 9.36	Α	C
ATOM	5350	C	MET	689	70. 897	69.539	50.479	1.00 17.90	Α	C
ATOM	5351	0	MET	689	71. 721	69. 220	51.341	1.00 16.90	Α	0
ATOM	5352	N	SER		70. 179		50.569	1.00 18.32	A	N
ATOM	5353	CA	SER		70. 358		51.712		Α	C
ATOM	5354	CB	SER	690	69. 621	72.866	51.501	1.00 20.29	Α	C
ATOM	5355	0G	SER	690	68. 234		51.711	1.00 24.78	A	0
ATOM	5356	C	SER	690	69. 898		53.038	1.00 22.31	Α	C
ATOM	5357	0	SER	690	69. 930	71.606	54.063	1.00 23.43	Α	0
ATOM	5358	N	ARG	691	69. 480	69.672	53.023	1.00 21.70	Α	N
ATOM	5359	CA	ARG	691	69. 041	69.012	54.249	1.00 23.07	Α	C
ATOM	5360	CB	ARG	691	67. 591	68. 546	54.113	1.00 22.90	A	C
ATOM	5361	CG	ARG	691	66. 623	69.652	53.770	1.00 22.81	A	C
ATOM	5362	CD	ARG	691	65. 201	69. 152	53.813	1.0022.97	Α	C
ATOM	5363	NE	ARG	691	64. 236	70. 240	53.694	1.00 24.03	Α	N
ATOM	5364	CZ	ARG	691	62. 963	70.134	54.061	1.00 26.18	A	C
ATOM	5365		ARG	691	62.509	68. 989	54.566	1.00 25.20	Α	N
ATOM ATOM	5366		ARG	691	62.149	71. 172	53.946	1.00 26.01	Α	N
ATOM	5367	C	ARG	691	69. 922	67.811	54. 593	1.00 24.24	Α	C
ATOM	5368	0 NT	ARG	.691	69. 595	67.031	55.488	1.00 25.28	A	0
ATOM	5369 5370	N	ALA	692	71.041	67.675	53.889	1.00 24.03	A	N
ATOM	5371	CA CB	ALA	692	71.960	66.561	54.100	1.00 24.84	A	C
ATOM	5372	CB	ALA	692	73. 270	66.826	53.360	1.00 24.20	Α	C
ATOM	5373	0	ALA ALA	692	72. 251	66. 210	55. 562	1.00 24.60	A	С
ATOM	5374	N	GLU	692	72.066	65.068	55.967	1.00 24.83	A	0
ATOM	5375	CA	GLU	693 693	72. 707	67. 181	56.347	1.00 25.74	A	N
ATOM	5376	CB	GLU	693	73.033	66. 944	57. 757	1.00 27.13	A	C
ATOM	5377	CG	GLU	693	73.351	68. 266	58. 463	1.00 29.38	A	Ċ
ATOM	5378	CD	GLU	693	74.829	68.606	58. 583	1.00 35.02	A	C
ATOM	5379		GLU	693	75. 604	67. 627	59.463	1.00 39.06	A	<u>C</u> .
ATOM	5380		GLU	693	74. 984	66.948	60.316	1.00 38.42	A	.0
ATOM	5381	C	GLU	693	76.845	67.554	59. 307	1.00 41.03	A	0
ATOM	5382	Õ	GLU	693	71. 947 72. 250	66. 215	58. 549	1.00 26.16	A	C
ATOM	5383	N	ASN	694	70.688	65. 505	59.506	1.00 26.78	A	0
ATOM	5384	CA	ASN	694	69. 594	66. 387 65. 734	58.160	1.00 24.46	A	N
ATOM	5385	CB	ASN	694	68. 274	66. 473	58.873	1.00 24.35	A	C
ATOM	5386	CG	ASN	694	68. 191	67. 796	58. 619 50. 270	1.00 26.79	A	C
ATOM	5387	0D1		694	67. 291	68. 607	59. 370 50. 122	1.00 28.23	A	C
ATOM	5388	ND2		694	69. 127	68. 015	59. 132 60. 287	1.00 29.60 1.00 27.09	A	0
ATOM	5389	C	ASN	694	69. 412	64. 252	58. 567	1.00 27.09	A	N
		-			UU. TI L	UT. 4U4	00.001	1.00 44.10	Α	С

					FIC	G. 4-	111			(Cont	tinued)
ATOM	5390	0	ASN	694	68.736	63.555	59. 318	1.00 22.09	A	0	
ATOM	5391	N	PHE	695	70.008	63.764		1.00 21.23	A	N	
ATOM	5392	CA	PHE	695	69.876	62.351	57. 135	1.00 20.87	A	C	
ATOM	5393	CB	PHE	695	70. 297	62.085		1.00 18.97	Α	С	
ATOM	5394	CG	PHE	695	69.262		54.663	1.00 15.41	A	C	
ATOM	5395		PHE	695	68. 980			1.00 16.20	Α	C	
ATOM	5396		PHE	695	68. 582			1.00 13.85	Α	C	
ATOM	5397		PHE	695	68. 033			1.00 15.80	A	C	
ATOM	5398		PHE	695	67. 636		52.976	1.00 14.69	A	C	
ATOM	5399	CZ	PHE	695	67. 360		52.710	1.00 14.36	A	C	
ATOM	5400	C	PHE	695	70. 704		58.068	1.00 22.60	A	C	
ATOM	5401	0	PHE	695	70. 734		57. 932	1.00 22.75	Α	0	
ATOM	5402	N	LYS	696	71.388	62.111	59.014	1.00 23.86	Α	N	
ATOM	5403	CA	LYS	696	72. 189	61.369	59. 980	1.00 24.30	Α	C	
ATOM	5404	CB	LYS	696	73. 119	62. 315	60.744	1.00 23.88	A	C	
ATOM	5405	CG	LYS	696	74. 230	62.883	59. 891	1.00 27.19	A	С	
ATOM	5406	CD	LYS	696	75. 160	63. 793	60.672	1.00 26.74	A	C	
ATOM	5407	CE	LYS	696	76. 354	64. 211	59.816	1.00 26.44	A	C	
ATOM	5408	NZ	LYS	696	77. 248	65. 163	60.534	1.00 28.88	A	N	
ATOM	5409	C	LYS	696	71. 256	60.670	60.962	1.00 24.58	A	C	
ATOM	5410	0	LYS	696	71.673	59. 790	61.710	1.00 24.47	A	0	
ATOM	5411	N	GLN	697	69. 986	61.060	60. 949	1.00 24.66	A	N	
ATOM	5412	CA	GLN	697	69.013	60. 476	61.865	1.00 26.18	A	C	
ATOM	5413	CB	GLN	697	68. 072	61.571	62. 385	1.00 28.53	A	C	
ATOM	5414	CG	GLN	697	68. 766	62. 865	62. 792	1.00 31.73	A	C	
ATOM	5415	CD	GLN	697	67. 790	63: 938	63. 262	1.00 34.90	A	C	
ATOM	5416	OE1		697	68. 086	65. 133	63. 195	1.00 37.16	A.	0	
ATOM	5417		GLN	697	66. 627	63. 516	63. 753	1.00 36.42	A	N	
ATOM ATOM	5418 5410	C	GLN	697	68. 176	59. 346	61. 259	1.00 24.79	A	C	
ATOM	5419 5420	0 M	GLN VAL	697	67. 294	58. 808	61.923	1.00 27.00	A	0	
ATOM	5420 5421	N Ca		698	68. 439	58. 979	60.011	1.00 21.46	A	N	
ATOM	5422	CB	VAL VAL	698 698	67.659	57. 922	59. 383	1.00 18.56	A	C	•
ATOM	5423		VAL	698	66. 510 65. 674	58. 517	58. 524	1.00 19.77	A	C	
ATOM	5424		VAL	698		59. 467 59. 233	59. 355	1.00 19.11	A	C	
ATOM	5425	C	VAL	698	68. 469	56. 987		1.00 15.74	A	. C	
ATOM	5426	Õ	VAL	698	69.614	57. 265	58. 484	1.00 18.57 1.00 17.50	A	C	
ATOM	5427	N	GLU	699	67. 850	55. 868	58. 135 58. 121		A	0	
ATOM	5428	CA	GLU	699	68.456	54. 885	57. 236	1.00 18.32 1.00 18.24	A	N	
ATOM	5429	CB	GLU	699	68.007	53. 488	57. 636	1.00 18.24	A	C	
ATOM	5430	CG	GLU	699	67.600	53. 411	59.097	1.00 15.38	A A	C	
ATOM	5431	CD	GLU	699	68.384	52. 377	59. 891	1.00 20.16	A	C	
ATOM	5432	0E1		699	69. 620	52. 305	59. 712	1.00 23.51	A	Ö	
ATOM	5433	0E2		699	67. 765	51.651	60. 703	1.00 31.31	A	0	
ATOM	5434	C	GLU	699	67.857	55. 286	55. 891	1.00 30.20	A	C	
ATOM	5435	ŏ	GLU	699	66.638	55. 397	55. 765	1.00 17.20	A	0	
ATOM	5436	N	TYR	700	68.714	55. 516	54. 899	1.00 15.53	A	N	
ATOM	5437	CA	TYR	700	68. 275	55. 968	53. 584	1.00 12.51	A	C	
ATOM	5438	CB	TYR	700	68.810	57. 383	53. 365	1.00 12.01	A	C	
					00.			1,00 10.00	11	U	

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					FIC	G. 4-	112	}		(Continue	d)
ATOM	5439	CG	TYR	700	68. 374	58. 105	52.114	1.00 13.03	A	С	
ATOM	5440		TYR	700	67.027	58. 171	51.746		Ä	č	
ATOM	5441		TYR	700	66. 611	58. 961	50.666		A	Č	
ATOM	5442		TYR	700	69. 301	58. 840	51.359		A	Č	
ATOM	5443		2 TYR	700	68. 895	59.629	50. 282		Ä	č	
ATOM	5444		TYR	700	67. 550	59.688	49.948		A	č	
ATOM	5445	0H	TYR	700	67. 150	60. 495	48.913		Ä	ŏ	
ATOM	5446	C	TYR	700	68. 743	55.056	52.468		Ä	č	
ATOM	5447	0	TYR	700	69. 881	54. 594	52.463		Ä	ŏ	
ATOM	5448		LEU	701	67.836	54.775	51.540	1.00 11.32	Ä	Ň	
ATOM	5449	CA	LEU	701	68.142	53.950	50.383	1.00 11.03	A	Ĉ	
ATOM	5450	CB	LEU	701	67. 313	52.667	50.378	1.00 8.96	Ā	Č	
ATOM	5451	CG	LEU	701	67.439	51.794	49.123	1.00 10.04	Ā	Č	
ATOM	5452	CD1	LEU	701	68.841	51.873	48.511	1.00 7.25	Ä	Č	
ATOM	5453	CD2	LEU	701	67.089	50.376	49.490	1.00 5.44	Ā	Č	
ATOM	5454	C	LEU	701	67.811	54. 799	49.170	1.00 13.03	A	Č	
ATOM	5455	0	LEU	701	66.660	55. 219	48.986	1.00 13.35	Α	0	
ATOM	5456	N	LEU	702	68.840	55.068	48.367	1.00 12.91	A	N	
ATOM	5457	CA	LEU	702	68. 724	55.888	47.169	1.00 11.74	Α	С	
ATOM	5458	CB	LEU	702	69.806	56.968	47.196	1.00 11.17	Α	С	
ATOM	5459	CG	LEU	702	69.916	57.965	46.044	1.00 12.13	Α	C	
ATOM	5460		LEU	702	68.569	58. 656	45.803	1.00 10.71	A	С	
ATOM	5461		LEU	702	71.006	58. 981	46.368	1.00 10.37	Α	C	
ATOM	5462	C	LEU	702	68. 883	55.003	45.942	1.00 13.49	Α	C	
ATOM	5463	0	LEU	702	69.854	54. 251	45.832	1.00 14.04	Α	0	
ATOM	5464	N	ILE	703	67. 935	55. 111	45.016	1.00 13.82	A	N	
ATOM	5465	CA	ILE	703	67. 934	54. 297	43.806	1.00 12.92	A	C	
ATOM ATOM	5466	CB	ILE	703	66. 931	53. 152	43.964	1.00 12.98	A	C	
ATOM	5467 5468		ILE	703	66.897	52. 305	42.706	1.00 15.12	A	C	
ATOM	5469	CD1	ILE ILE	703	67. 299	52. 322	45. 196	1.00 13.52	A	C	
ATOM	5470	CDI	ILE	703 703	66. 202	51.383	45.663	1.00 13.28	A	C	
ATOM	5471	0	ILE	703 703	67. 561 66. 635	55. 125 55. 938	42.582	1.00 14.12	A	C	
ATOM	5472	N	HIS	703 704	68. 265	50. 938 54. 909	42.629 41.473	1.00 15.85	A	0	
ATOM	5473	CA	HIS	704	67. 987	55. 678	40. 265	1.00 13.28	A	N	
ATOM	5474	CB	HIS	704	68. 670	57. 048	40. 203	1.00 11.81 1.00 11.13	A	C	
ATOM	5475		HIS	704	67. 968	58. 156	39.667	1.00 11.13	A	C	
ATOM	5476		HIS	704	67.446	58. 221	38. 418	1.00 11.00	A A	C C	
ATOM	5477		HIS	704	67.736	59. 387	40. 244	1.00 10.03	A	N	
ATOM	5478		HIS	704	67.098	60. 162	39. 385	1.00 9.04	A	C	
ATOM	5479		HIS	704	66.910	59.479	38. 270	1.00 11.23	A	N	
ATOM	5480	C	HIS	704	68.464	54.965	38. 992	1.00 11.87	A	C	
ATOM	5481	0	HIS	704	69.503	54. 306	38. 980	1.00 11.87	A	0	
ATOM	5482	N	GLY	705	67. 684	55.082	37. 926	1.00 11.49	A	N	
ATOM	5483	CA	GLY	705	68.075	54.486	36.663	1.00 11.90	Ä	Č	
ATOM	5484	C	GLY	705	69.066	55.449	36.036	1.00 12.16	Ä	Č	
ATOM	5485	0	GLY	705	68. 911	56.660	36. 153	1.00 13.94	Ā	Ŏ	
ATOM	5486	N	THR	706	70.086	54.928	35. 372	1.00 13.29	Ä	N	•
ATOM	5487	CA	THR	706	71.101	55. 782	34. 770	1.00 12.51	A	C	

			FIG. 4-113	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	5488 CB TH 5489 OG1 TH 5490 CG2 TH 5491 C TH 5492 O TH 5493 N AL 5494 CA AL 5495 CB AL 5496 C AL 5497 O AL 5498 N AS 5499 CA AS 5500 CB AS	R 706 R 706 R 706 R 706 A 707 P 708 P 708	72. 417 55. 001 34. 557 1. 00 11. 94 A 72. 230 53. 983 33. 565 1. 00 12. 79 A 72. 840 54. 344 35. 861 1. 00 12. 66 A 70. 678 56. 409 33. 455 1. 00 13. 02 A 71. 183 57. 461 33. 084 1. 00 14. 35 A 69. 754 55. 770 32. 748 1. 00 13. 82 A 69. 289 56. 302 31. 469 1. 00 15. 26 A 69. 126 55. 176 30. 442 1. 00 13. 60 A 67. 970 57. 030 31. 644 1. 00 16. 56 A 67. 154 57. 075 30. 720 1. 00 17. 71 A 67. 764 57. 600 32. 828 1. 00 16. 33 A 66. 534 58. 314 33. 113 1. 00 16. 71 A	C O C C O N C C C O N
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	5501 CG ASI 5502 OD1 ASI 5503 OD2 ASI 5504 C ASI 5505 O ASI 5506 N ASI 5507 CA ASI	708 708 708 708 708 708 709	64. 957 58. 834 35. 000 1. 00 19. 59 A 64. 304 59. 612 34. 266 1. 00 18. 82 A 64. 498 58. 317 36. 038 1. 00 19. 68 A 66. 490 59. 673 32. 408 1. 00 17. 30 A 67. 131 60. 647 32. 843 1. 00 18. 75 A 65. 715 59. 722 31. 327 1. 00 13. 98	C C O O C O N
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	5508 CB ASP 5509 CG ASP 5510 OD1 ASP 5511 OD2 ASP 5512 C ASP 5513 O ASP 5514 N ASN	709 709 709 709 709 709	65. 553 60. 913 30. 509 1. 00 13. 26 A 65. 028 60. 503 29. 137 1. 00 11. 83 A 63. 700 59. 778 29. 228 1. 00 13. 61 A 62. 648 60. 402 28. 958 1. 00 12. 39 A 63. 706 58. 584 29. 593 1. 00 10. 85 A 64. 603 61. 934 31. 129 1. 00 13. 44 A 64. 649 63. 112 30. 786 1. 00 14. 33 A 63. 743 61. 473 32. 034 1. 00 12. 40	C C O O C O N
ATOM ATOM ATOM ATOM ATOM ATOM	5515 CA ASN 5516 CB ASN 5517 CG ASN 5518 OD1 ASN 5519 ND2 ASN 5520 C ASN 5521 O ASN	710 710 710 710 710 710 710 710	62. 761 62. 331 32. 702 1. 00 11. 63 A 61. 566 61. 469 33. 094 1. 00 10. 91 A 60. 388 62. 276 33. 572 1. 00 12. 77 A 59. 271 61. 760 33. 651 1. 00 14. 18 A 60. 621 63. 539 33. 903 1. 00 12. 05 A 63. 395 63. 010 33. 938 1. 00 13. 10 A 63. 691 64. 211 33. 912 1. 00 12. 53 A	C C C O N C
ATOM ATOM ATOM ATOM ATOM ATOM	5522 N VAL 5523 CA VAL 5524 CB VAL 5525 CG1 VAL 5526 CG2 VAL 5527 C VAL 5528 O VAL	711 711 711 711 711 711 711	63. 570 62. 246 35. 017 1. 00 11. 10 A 64. 221 62. 741 36. 225 1. 00 9. 96 A 63. 620 62. 128 37. 512 1. 00 9. 85 A 64. 415 62. 570 38. 719 1. 00 7. 61 A 62. 176 62. 567 37. 675 1. 00 11. 26 A 65. 645 62. 237 36. 038 1. 00 10. 48 A 65. 949 61. 068 36. 280 1. 00 10. 00 A	N C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	5529 N HIS 5530 CA HIS 5531 CB HIS 5532 CG HIS 5533 CD2 HIS 5534 ND1 HIS 5535 CE1 HIS 5536 NE2 HIS	712 712 712 712 712 712 712 712 712	66. 518 63. 126 35. 591 1. 00 10. 94 A 67. 899 62. 758 35. 302 1. 00 11. 74 A 68. 577 63. 961 34. 646 1. 00 10. 79 A 67. 782 64. 529 33. 514 1. 00 11. 58 A 66. 855 63. 955 32. 705 1. 00 12. 39 A 67. 833 65. 858 33. 154 1. 00 11. 87 A 66. 966 66. 082 32. 181 1. 00 12. 19 A 66. 359 64. 944 31. 891 1. 00 11. 62	N C C C C N C

			FIG. 4-114	(Continued)
ATOM 5 AT	537 C HIS 538 O HIS 539 N PHE 540 CA PHE 541 CB PHE 542 CG PHE 542 CG PHE 544 CD2 PHE 544 CD2 PHE 545 CE1 PHE 546 CE2 PHE 547 CZ PHE 548 C PHE 549 O PHE 550 N GLN 551 CA GLN 551 CA GLN 551 CA GLN 552 CB GLN 553 CG GLN 555 OE1 GLN 555 OE1 GLN 555 OE1 GLN 556 NE2 GLN 556 NE2 GLN 566 C GL	712 713 713 713 713 713 713 713 713 713	68. 698 62. 222 36. 491 1. 00 10. 63 A 68. 461 62. 598 37. 633 1. 00 11. 98 A 69. 631 61. 319 36. 210 1. 00 10. 82 A 70. 458 60. 720 37. 251 1. 00 11. 00 A 71. 533 59. 823 36. 634 1. 00 11. 14 A 72. 270 58. 989 37. 639 1. 00 11. 47 A 71. 714 57. 813 38. 126 1. 00 11. 22 A 73. 496 59. 407 38. 144 1. 00 11. 84 A 72. 367 57. 066 39. 109 1. 00 11. 98 A 74. 153 58. 667 39. 126 1. 00 13. 82 A 73. 586 57. 495 39. 610 1. 00 11. 85 A 71. 404 61. 640 39. 243 1. 00 13. 14 A 71. 377 62. 948 37. 403 1. 00 12. 47 A 72. 001 64. 113 38. 022 1. 00 10. 55 A 71. 851 65. 321 37. 082 1. 00 11. 91 A 72. 055 66. 695 37. 740 1. 00 10. 69 A 71. 501 67. 827 36. 891 1. 00 9. 77 A 70. 447 67. 693 36. 268 1. 00 10. 50 A 72. 201 68. 948 36. 870 1. 00 9. 91 A 72. 037 64. 700 40. 356 1. 00 8. 86 A 70. 029 64. 340 39. 395 1. 00 10. 27 A 69. 255 64. 616 40. 599 1. 00 10. 98 A 67. 267 65. 219 39. 144 1. 00 11. 10 A 66. 285 66. 288 39. 567 1. 00 12. 90 A 69. 716 63. 781 41. 780 1. 00 10. 65 A 66. 381 66. 828 40. 671 1. 00 10. 65 A 66. 381 66. 828 40. 671 1. 00 10. 65 A 66. 381 66. 828 40. 671 1. 00 10. 65 A 66. 381 66. 828 40. 671 1. 00 10. 65 A 66. 381 66. 828 40. 671 1. 00 10. 65 A 66. 381 66. 828 40. 671 1. 00 10. 65 A 69. 976 64. 322 42. 853 1. 00 12. 32 A 69. 828 62. 472 41. 600 1. 00 9. 91	
ATOM 55 ATOM 55	70 CB SER 71 OG SER	716 716	69. 937 60. 163 42. 461 1. 00 10. 77 A 68. 541 59. 994 42. 492 1. 00 14. 60 A	C C O
ATOM 55 ATOM 55 ATOM 55 ATOM 55	73 0 SER 74 N ALA 75 CA ALA	716 716 717 717	71. 818 61. 761 42. 876 1. 00 13. 46 A 72. 341 61. 556 43. 976 1. 00 14. 90 A 72. 522 62. 094 41. 797 1. 00 12. 22 A 73. 969 62. 252 41. 870 1. 00 13. 92 A	C O N C
ATOM 55' ATOM 55' ATOM 55' ATOM 55' ATOM 55' ATOM 558 ATOM 558	77 C ALA 78 O ALA 79 N GLN 80 CA GLN	717 717 717 718 718	74. 555 62. 487 40. 479 1. 00 12. 46 A 74. 299 63. 423 42. 790 1. 00 13. 73 A 75. 257 63. 375 43. 560 1. 00 15. 24 A 73. 504 64. 482 42. 710 1. 00 13. 27 73. 738 65. 631 43. 565 1. 00 13. 07 A	C C O N C
ATOM 558 ATOM 558 ATOM 558 ATOM 558 ATOM 558	82 CG GLN 83 CD GLN 84 OE1 GLN	718 718 718 718 718	72. 976 66. 841 43. 035 1. 00 13. 93 A 73. 548 67. 422 41. 734 1. 00 15. 44 A 74. 996 67. 865 41. 867 1. 00 13. 84 A 75. 467 68. 172 42. 950 1. 00 16. 85 A 75. 699 67. 915 40. 755 1. 00 17. 86 A	C C C O N

ATOM 5588 C C CLN 718	ATOM 5587 O GLN 718 73.941 65.910 45.949 1.00 11.74 A 0 ATOM 5588 N ILE 719 72.370 64.460 45.237 1.00 12.01 A N ATOM 5590 CB ILE 719 70.691 63.201 46.616 1.00 12.50 A C ATOM 5592 CG1 ILE 719 70.464 62.673 48.021 1.00 11.09 A C ATOM 5593 CD1 ILE 719 69.447 63.979 46.174 1.00 14.37 A C ATOM 5594 C ILE 719 73.081 63.338 47.282 1.00 11.72 A C ATOM 5595 O ILE 719 73.081 63.338 47.282 1.00 11.72 A C ATOM 5596 N SER 720 73.508 62.262 46.632 1.00 11.35 A N ATOM 5597 CA SER 720 74.557 61.405 47.155 1.00 11.02 A C ATOM 5599 OG SER 720 74.557 61.405 47.155 1.00 11.02 A C ATOM 5599 OG SER 720 75.471 60.894 44.970 1.00 13.75 A O ATOM 5600 C SER 720 75.804 62.207 47.488 1.00 12.63 A C ATOM 5601 O SER 720 76.429 61.995 48.537 1.00 11.68 A O ATOM 5603 CA LYS 721 77.336 63.951 46.800 1.00 12.15 A C ATOM 5604 CB LYS 721 77.336 63.951 46.800 1.00 12.15 A C ATOM 5605 CG LYS 721 77.316 64.823 45.571 1.00 11.24 A C ATOM 5605 CG LYS 721 77.316 66.844 44.4551 1.00 12.18 A N A C ATOM 5605 CG LYS 721 77.517 66.064 44.4551 1.00 12.18 A O A C ATOM 5605 CG LYS 721 77.517 66.064 44.4551 1.00 12.18 A O A C ATOM 5605 CG LYS 721 77.517 66.064 44.4551 1.00 12.24 A C ATOM 5605 CG LYS 721 77.517 66.064 44.4551 1.00 12.24 A C ATOM 5605 CG LYS 721 77.517 66.064 44.4551 1.00 12.24 A C ATOM 5605 CG LYS 721 77.517 66.064 44.4551 1.00 12.24 A C ATOM 5605 CG LYS 721 77.517 66.064 44.4551 1.00 12.24 A C ATOM 5605 CG LYS 721 77.517 66.064 44.4551 1.00 12.24 A C ATOM 5606 CD LYS 721 77.517 66.064 44.4551 1.00 12.18 A O A C ATOM 5606 CD LYS 721 77.517 66.064 44.4551 1.00 12.24 A C ATOM 5606 CD LYS 721 77.517 66.064 44.4551 1.00 12.24 A C ATOM 5606 CD LYS 721 77.517 66.064 44.4551 1.00 12.24 A C ATOM 5606 CD LYS 721 77.517 66.064 44.4551 1.00 12.24 A C ATOM 5606 CD LYS 721 77.517 66.064 44.4551 1.00 12.24 A C ATOM 5606 CD LYS 721 77.517 66.064 44.4551 1.00 12.24 A C ATOM 5606 CD LYS 721 77.517 66.064 44.4551 1.00 12.24 A C ATOM 5606 CD LYS 721 77.517 66.064 44.4551 1.00 12.24 A C ATOM 5606 CD LYS 721 77.517 66.064 44.4551 1.00 12.24 A C ATOM 5606 CD LYS 721
ATOM 5633 CB ASP 725 79. 627 67. 032 50. 919 1. 00 22. 40 A C	ATOM 5607 CE LYS 721 78.674 66.765 43.392 1.00 8.74 A C ATOM 5608 NZ LYS 721 78.341 68.165 43.739 1.00 9.54 A N ATOM 5609 C LYS 721 77.190 64.816 48.038 1.00 13.24 A C ATOM 5610 0 LYS 721 78.150 64.982 48.791 1.00 14.49 A 0 ATOM 5611 N ALA 722 75.992 65.351 48.262 1.00 13.05 A N ATOM 5613 CB ALA 722 75.760 66.198 49.432 1.00 13.21 A C ATOM 5613 CB ALA 722 75.874 65.369 50.702 1.00 14.04 A C ATOM 5615 O ALA 722 75.874 65.369 50.702 1.00 14.04 A C ATOM 5616 N LEU 723 75.360 64.145 50.665 1.00 14.96 A N ATOM 5617 CA LEU 723 75.429 63.266 51.826 1.00 17.23 A C ATOM 5618 CB LEU 723 74.626 61.984 51.570 1.00 16.86 A C ATOM 5621 CD2 LEU 723 73.116 62.205 51.463 1.00 18.78 A C ATOM 5620 CD1 LEU 723 77.320 62.990 53.280 1.00 18.74 A C ATOM 5623 O LEU 723 77.320 62.990 53.280 1.00 18.48 A O ATOM 5624 N VAL 724 77.641 62.559 51.103 1.00 17.26 A C ATOM 5626 CB VAL 724 79.671 61.824 49.902 1.00 14.31 A C ATOM 5627 CG1 VAL 724 79.671 61.824 49.902 1.00 14.31 A C ATOM 5628 CG2 VAL 724 79.671 61.824 49.902 1.00 14.31 A C ATOM 5628 CG2 VAL 724 79.671 61.824 49.902 1.00 14.31 A C ATOM 5630 O VAL 724 79.871 61.824 49.902 1.00 14.31 A C ATOM 5631 N ASP 725 79.411 64.632 51.318 1.00 19.19 A N ATOM 5632 CA ASP 725 80.051 65.848 51.776 1.00 19.09 A O ATOM 5633 CB ASP 725 80.051 65.848 51.776 1.00 19.09 A O ATOM 5633 CB ASP 725 80.051 65.848 51.776 1.00 19.09 A O ATOM 5633 CB ASP 725 80.051 65.848 51.776 1.00 19.09 A O ATOM 5633 CB ASP 725 80.051 65.848 51.776 1.00 19.09 A O ATOM 5633 CB ASP 725 80.051 65.848 51.776 1.00 19.09 A O ATOM 5633 CB ASP 725 80.051 65.848 51.776 1.00 19.09 A O ATOM 5633 CB ASP 725 80.051 65.848 51.776 1.00 20.26 A C

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	٠.				FIC	. 4 -	1 1 6			(Con	tinued)
ATOM ATOM	5635 5636		ASP ASP	725 725	81. 149 79. 867	66. 151 67. 839	49.319 48.704	1.00 26.28 1.00 30.70	A A	0	
ATOM	5637	C	ASP	725	79.805	66.171	53. 238	1.00 19.86	Α	C	
ATOM	5638	0	ASP	725	80. 486	67. 024	53.792	1.00 23.33	A	0 N	
ATOM ATOM	5639 5640	N CA	VAL VAL	726 726	78. 841 78. 603	65. 516 65. 790	53.873 55.285	1.00 17.95 1.00 17.97	A A	N C	
ATOM	5641	CB	VAL	726	77. 178	66. 341	55. 567	1.00 18.54	A	Č	
ATOM	5642		VAL	726	76. 992	67. 680	54.875	1.00 16.64	Ä	č	
ATOM	5643		VAL	726	76. 121	65. 339	55.120	1.00 18.24	A	C	
ATOM	5644	C	VAL	726	78.812	64. 549	56.124	1.00 17.82	Α	C	
ATOM	5645	0	VAL	726	78.412	64. 504	57. 283	1.00 19.86	A	0	
ATOM	5646	N	GLY	727	79.439	63. 541	55.535	1.00 17.13	A	N	
ATOM	5647	CA	GLY	. 727	79.711	62.317	56. 263	1.00 16.84	` A	C	
ATOM ATOM	5648 5649	C 0	GLY GLY	727 727	78. 509 78. 483	61. 489 60. 961	56.681 57.794	1.00 17.94 1.00 19.74	A A	C 0	
ATOM	5650	N	VAL	728	77. 517	61. 371	55.802	1.00 16.62	A	N	
ATOM	5651	CA	VAL	728	76. 331	60. 571	56.085	1.00 17.26	Ä	Ċ	•
ATOM	5652	CB	VAL	728	75.030	61.302	55.643	1.00 18.46	A	Č	
ATOM	5653		VAL	728 .	73.838	60.338	55.668	1.00 16.22	Α	C	
ATOM	5654		VAL	728	74. 753	62.476	56.579	1.00 18.70	Α	C	
ATOM	5655	C	VAL	728	76.411	59. 230	55.347	1.00 18.03	A	C	
ATOM	5656	0	VAL	728	76.667	59. 186	54.143	1.00 18.40 -	A	0	
ATOM	5657	N	ASP	729	76. 211	58. 135	56.069	1.00 18.22	A	N	
ATOM ATOM	5658 5659	CA CB	ASP ASP	729 729	76. 246 76. 734	56. 822 55. 752	55. 441 56. 420	1.00 19.90 1.00 22.57	A A	C	
ATOM	5660	CG	ASP	729	76. 819	54. 376	55. 778	1.00 25.97	A A	C C	
ATOM	5661		ASP	729	77. 340	54. 278	54.649	1.00 27.13	A	Õ	
ATOM	5662		ASP	729	76. 372	53. 388	56.398	1.00 30.03	Ä	ŏ	
ATOM -	5663	C	ASP	729	74.839	56. 504	54.984	1.00 19.16	Ä	Č	
ATOM	5664	0	ASP	729	73.868	56.863	55.649	1.00 21.91	Α	0	
ATOM	5665	N	PHE	730	74. 723	55. 838	53.846	1.00 18.27	Α	N	
ATOM	5666	CA	PHE	730	73.416	55. 499	53. 299	1.00 16.06	A	Ç	
ATOM	5667	CB	PHE	730	72. 796	56. 734	52.639	1.00 14.49	A	C	
ATOM ATOM	5668 5669	CC	PHE PHE	730 730	73. 590 73. 262	57. 265 56. 913	51.480 50.177	1.00 12.02	A	C	
ATOM	5670		PHE	730	74. 691	58. 082	51.694	1.00 10.26 1.00 11.55	A A	C C	
ATOM	5671		PHE	730	74. 020	57. 364	49.098	1.00 10.41	A	Č	
ATOM	5672		PHE	730	75. 459	58. 537	50.621	1.00 13.40	A	č	
ATOM	5673	CZ	PHE	730	75.120	58. 175	49.317	1.00 9.85	A	Č	
ATOM	5674	C	PHE	730	73.565	54. 388	52.281	1.00 16.20	Α	C	
ATOM	5675	0	PHE	730	74.675	53. 990	51.945	1.00 18.49	A	0	
ATOM	5676	N	GLN	731	72.447	53. 883	51.791	1.00 17.40	A	N	
ATOM	5677	CA	GLN	731	72. 484	52.813	50.813	1.00 17.82	A	. C	
ATOM ATOM	5678 5679	CB CG	GLN GLN	731 731	71.514	51.708 51.257	51.208 52.644	1.00 20.04 1.00 25.37	A A	C C	
ATOM -	5680	CD	GLN	731	71.641 73.019	50. 737	52. 968	1.00 25.37	A A	C	
ATOM	5681		GLN	731	73. 554	49. 883	52. 256	1.00 32.85	A	Ö	
ATOM	5682		GLN	731	73. 603	51. 238	54.055	1.00 30.12	Ä	N	
ATOM	5683	C	GLN	731	72. 091	53. 382	49.458	1.00 17.65	Ä	Ċ	

			FIG. 4-117	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	M 5685 N AL M 5686 CA AL M 5687 CB AL M 5688 C AL M 5689 O AL M 5690 N ME M 5691 CA ME M 5692 CB ME M 5692 CB ME M 5693 CG ME M 5694 SD ME M 5695 CE ME M 5695 CE ME M 5696 C ME M 5697 O ME M 5698 N TRP M 5699 CA TRP M 5700 CB TRP M 5700 CB TRP M 5701 CG TRP M 5701 CG TRP M 5702 CD2 TRP M 5703 CE2 TRP M 5704 CE3 TRP M 5705 CD1 TRP M 5705 CD1 TRP M 5706 NE1 TRP	A 732 A 732 A 732 A 732 A 732 A 733 A 733 A 733 A 733 A 733 A 733 A 734 A 735 A 735	71. 160 54. 191 49. 355 1. 00 17. 02 A 72. 802 52. 962 48. 421 1. 00 14. 78 A 72. 510 53. 444 47. 088 1. 00 15. 21 A 73. 588 54. 409 46. 626 1. 00 15. 17 A 72. 419 52. 282 46. 131 1. 00 15. 21 A 72. 940 51. 207 46. 396 1. 00 16. 17 A 71. 737 52. 504 45. 019 1. 00 14. 57 A 71. 599 51. 483 44. 008 1. 00 14. 86 A 70. 490 50. 499 44. 383 1. 00 15. 14 A 70. 288 49. 386 43. 353 1. 00 18. 04 A 71. 814 48. 476 42. 961 1. 00 22. 04 A 71. 892 47. 307 44. 310 1. 00 17. 75 A 71. 283 52. 153 42. 683 1. 00 14. 93 A 70. 317 52. 915 42. 574 1. 00 13. 98 A 72. 113 51. 884 41. 680 1. 00 13. 82 A 71. 890 52. 447 40. 356 1. 00 13. 13 A 73. 173 53. 117 39. 827 1. 00 10. 39 A 74. 187 52. 159 39. 267 1. 00 8. 77 A 75. 398 51. 726 39. 894 1. 00 7. 74 A 75. 984 50. 757 39. 053 1. 00 9. 97 76. 045 52. 062 41. 087 1. 00 8. 70 74. 095 51. 463 38. 095 1. 00 10. 56 A 75. 170 50. 613 37. 961 1. 00 12. 87	(Continued) O N C C C C O N C C C C C C C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	5705 CD1 TRP 5706 NE1 TRP 5707 CZ2 TRP 5708 CZ3 TRP 5709 CH2 TRP 5710 C TRP 5711 O TRP 5712 N TYR 5713 CA TYR 5714 CB TYR 5715 CG TYR 5716 CD1 TYR 5717 CE1 TYR 5718 CD2 TYR 5719 CE2 TYR 5720 CZ TYR	734	74. 095 51. 463 38. 095 1. 00 10. 56 A 75. 170 50. 613 37. 961 1. 00 12. 87 77. 183 50. 119 39. 369 1. 00 9. 94 A 77. 238 51. 428 41. 400 1. 00 9. 32 A 77. 793 50. 468 40. 545 1. 00 9. 49 A 71. 480 51. 291 39. 445 1. 00 14. 06 A 71. 903 50. 155 39. 653 1. 00 13. 91 A 70. 635 51. 570 38. 461 1. 00 15. 15 A 70. 223 50. 544 37. 504 1. 00 15. 51 A 68. 705 50. 326 37. 556 1. 00 14. 10 A 68. 300 49. 439 38. 709 1. 00 14. 76 A 68. 619 48. 081 38. 708 1. 00 14. 76 A 68. 360 47. 278 39. 816 1. 00 14. 33 A 67. 696 49. 971 39. 848 1. 00 15. 84 A 67. 432 49. 180 40. 960 1. 00 14. 52	C N C C C C C C C C C C C C C C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	5721 OH TYR 5722 C TYR 5723 O TYR 5724 N THR 5725 CA THR 5726 CB THR 5727 OG1 THR 5728 CG2 THR 5729 C THR 5730 O THR 5731 N ASP 5732 CA ASP	735 735 736 736 736 736 736 736 736 736 737	67. 772 47. 835 40. 938 1. 00 16. 33 A 67. 547 47. 056 42. 048 1. 00 17. 53 A 70. 685 50. 966 36. 104 1. 00 16. 31 A 70. 103 51. 858 35. 466 1. 00 15. 82 A 71. 763 50. 330 35. 654 1. 00 15. 44 A 72. 361 50. 608 34. 353 1. 00 15. 13 A 73. 491 49. 602 34. 030 1. 00 14. 68 A 74. 470 49. 614 35. 076 1. 00 15. 48 A 74. 156 49. 961 32. 713 1. 00 14. 72 A 71. 365 50. 549 33. 206 1. 00 15. 41 A 70. 650 49. 560 33. 044 1. 00 16. 44 A 71. 335 51. 614 32. 414 1. 00 15. 92 A 70. 475 51. 719 31. 238 1. 00 16. 48	C O C O C C C O N C

				FIG	G. 4	118			(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	5736 OD 5737 C 5738 O 5739 N 5740 CA 5741 CB 5742 CG 5743 CD 5744 OE 5745 OE 5746 C 5747 O 5748 N 5749 CA 5750 CB 5751 CG 5752 OD 5754 C 5755 CA 5757 CA 5758 CB	ASP ASP ASP ASP GLU GLU GLU GLU GLU GLU GLU ASP	737 737 737 737 737 738 738 738 738 738	70. 884 72. 232 72. 679 72. 847 68. 974 68. 205 68. 553 67. 135 66. 909 66. 904 65. 741 64. 588 65. 970 66. 624 67. 327 65. 414 64. 892 64. 074 62. 689 61. 995 62. 285 64. 088 64. 191 63. 291 62. 521 61. 746	50. 677 50. 972 50. 147 52. 020 51. 632 51. 507 51. 692 51. 644 50. 999 49. 485 48. 937 49. 289 48. 163 53. 076 53. 991 53. 288 54. 642 54. 863 54. 271 54. 340 53. 752 54. 976 54. 282 56. 034 56. 469 57. 736	30. 200 29. 574 28. 747 29. 895 31. 467 30. 515 32. 722 33. 033 34. 407 34. 380 33. 565 33. 878 32. 611 32. 525 32. 493 31. 222 31. 293 30. 257 32. 358 33. 750 34. 762 33. 687 34. 842 34. 511	1.00 15.90 1.00 20.37 1.00 24.29 1.00 18.74 1.00 17.71 1.00 18.39 1.00 19.00 1.00 20.24 1.00 20.93 1.00 24.58 1.00 27.21 1.00 26.16 1.00 19.38 1.00 20.83 1.00 19.38 1.00 21.35 1.00 21.35 1.00 21.35 1.00 16.96 1.00 18.24 1.00 16.96 1.00 16.88	A A A A A A A A A A A A A A A A A A A	C C C O O C C C C O O C C C C C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	5759 CG 5760 CD2 5761 ND1 5762 CE3 5763 NE2 5764 C 5765 O 5766 N 5767 CA 5768 C 5769 O 5770 N 5771 CA 5772 CB 5773 CG2 5774 CG1	HIS HIS HIS HIS HIS HIS GLY GLY GLY ILE ILE ILE ILE ILE ALA ALA ALA	740 740 740 740 740 740 741 741 741 741 742 742 742 742 742 742 742 743 743 743 743	61. 145 59. 883 61. 881 61. 097 59. 880 61. 557 61. 191 60. 216 60. 849 60. 165 62. 145 62. 854 63. 273 64. 279 63. 865 64. 540 61. 907 61. 805 61. 217 60. 246 59. 004 60. 717	58. 392 58. 812 58. 687 59. 262 59. 349 55. 539 54. 481 53. 484 52. 218 51. 404 52. 045 50. 849 50. 981 49. 917 52. 370 52. 552 49. 658 48. 825 49. 594 48. 538 49. 141 47. 350	35. 710, 35. 961, 36. 837, 732, 37. 224, 35. 426, 36. 599, 34. 614, 35. 609, 36. 237, 35. 368, 37. 294, 37. 638, 37. 540, 38. 887, 35. 676, 36. 571, 34. 534, 268, 33. 630	1. 00 10. 68 1. 00 17. 57 1. 00 16. 26 1. 00 17. 31 1. 00 18. 51 1. 00 19. 90 1. 00 20. 00 1. 00 19. 40 1. 00 18. 82 1. 00 20. 36 1. 00 22. 79 1. 00 19. 61 1. 00 17. 74 1. 00 14. 46 1. 00 14. 37 1. 00 13. 43 1. 00 9. 55 1. 00 19. 11 1. 00 18. 97 1. 00 20. 16 1. 00 19. 71 1. 00 19. 65 1. 00 20. 08	A A A A A A A A A A A A A A A A A A A	C C C N C N C C C C C C C C C C C C C C

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ATOM 5819 CB GLN 749 62. 408 40. 801 39. 519 1. 00 20. 05 A C ATOM 5820 CG GLN 749 61. 291 40. 428 38. 550 1. 00 21. 82 A C ATOM 5821 CD GLN 749 61. 618 39. 190 37. 757 1. 00 20. 87 A C ATOM 5822 OE1 GLN 749 62. 047 38. 187 38. 316 1. 00 22. 37 A O ATOM 5823 NE2 GLN 749 61. 415 39. 249 36. 447 1. 00 20. 00 A N ATOM 5824 C GLN 749 63. 416 42. 524 41. 008 1. 00 19. 07 A C ATOM 5825 O GLN 749 63. 335 42. 388 42. 231 1. 00 17. 88 A O ATOM 5826 N HIS 750 64. 508 42. 972 40. 399 1. 00 18.			CA	GLN								
ATOM 5820 CG GLN 749 61.291 40.428 38.550 1.00 21.82 A C ATOM 5821 CD GLN 749 61.618 39.190 37.757 1.00 20.87 A C ATOM 5822 OE1 GLN 749 62.047 38.187 38.316 1.00 22.37 A O ATOM 5823 NE2 GLN 749 61.415 39.249 36.447 1.00 20.00 A N ATOM 5824 C GLN 749 63.416 42.524 41.008 1.00 19.07 A C ATOM 5825 O GLN 749 63.335 42.388 42.231 1.00 17.88 A O ATOM 5826 N HIS 750 64.508 42.972 40.399 1.00 18.97 A N ATOM 5827 CA HIS 750 65.707 43.275 41.160 1.00 16.68 A C ATOM 5828 CB HIS 750 66.871 43.597 40.226 1.00 14.65 A C					749							
ATOM 5821 CD GLN 749 61.618 39.190 37.757 1.00 20.87 A C ATOM 5822 0E1 GLN 749 62.047 38.187 38.316 1.00 22.37 A 0 ATOM 5823 NE2 GLN 749 61.415 39.249 36.447 1.00 20.00 A N ATOM 5824 C GLN 749 63.416 42.524 41.008 1.00 19.07 A C ATOM 5825 O GLN 749 63.335 42.388 42.231 1.00 17.88 A 0 ATOM 5826 N HIS 750 64.508 42.972 40.399 1.00 18.97 A N ATOM 5827 CA HIS 750 65.707 43.275 41.160 1.00 16.68 A C ATOM 5828 CB HIS 750 66.871 43.597 40.226 1.00 14.65 A C						61.291 4						
ATOM 5822 OE1 GLN 749 62.047 38.187 38.316 1.00 22.37 A 0 ATOM 5823 NE2 GLN 749 61.415 39.249 36.447 1.00 20.00 A N ATOM 5824 C GLN 749 63.416 42.524 41.008 1.00 19.07 A C ATOM 5825 O GLN 749 63.335 42.388 42.231 1.00 17.88 A 0 ATOM 5826 N HIS 750 64.508 42.972 40.399 1.00 18.97 A N ATOM 5827 CA HIS 750 65.707 43.275 41.160 1.00 16.68 A C ATOM 5828 CB HIS 750 66.871 43.597 40.226 1.00 14.65 A C												
ATOM 5824 C GLN 749 63.416 42.524 41.008 1.00 19.07 A C ATOM 5825 O GLN 749 63.335 42.388 42.231 1.00 17.88 A O ATOM 5826 N HIS 750 64.508 42.972 40.399 1.00 18.97 A N ATOM 5827 CA HIS 750 65.707 43.275 41.160 1.00 16.68 A C ATOM 5828 CB HIS 750 66.871 43.597 40.226 1.00 14.65 A C									1.00	22.37		
ATOM 5825 O GLN 749 63.335 42.388 42.231 1.00 17.88 A O ATOM 5826 N HIS 750 64.508 42.972 40.399 1.00 18.97 A N ATOM 5827 CA HIS 750 65.707 43.275 41.160 1.00 16.68 A C ATOM 5828 CB HIS 750 66.871 43.597 40.226 1.00 14.65 A C											A	N
ATOM 5826 N HIS 750 64.508 42.972 40.399 1.00 18.97 A N ATOM 5827 CA HIS 750 65.707 43.275 41.160 1.00 16.68 A C ATOM 5828 CB HIS 750 66.871 43.597 40.226 1.00 14.65 A C												C
ATOM 5827 CA HIS 750 65.707 43.275 41.160 1.00 16.68 A C ATOM 5828 CB HIS 750 66.871 43.597 40.226 1.00 14.65 A C												
ATOM 5828 CB HIS 750 66.871 43.597 40.226 1.00 14.65 A C												
ATOM 5000 CC HIG 750												
111 111 111 111 111 111 11 11 11 11 11	ATOM	5829		HIS	750 750							
	ATOM											

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			FIG. 4-120	(Continued)
.=			116. 4-120	
ATOM ATOM	5831 ND1 H 5832 CE1 H		68. 615 44. 365 41. 877 1. 00 13. 54 A	
ATOM	5833 NE2 H		69. 804 44. 000 42. 320 1. 00 12. 57 A 70. 185 42. 927 41. 653 1. 00 12. 04 A	
ATOM		IS 750	05 500	
ATOM		IS 750	65. 529 44. 400 42. 157 1. 00 17. 33 A 65. 945 44. 277 43. 309 1. 00 18. 09 A	
ATOM	5836 N I	LE 751	64. 899 45. 490 41. 726 1. 00 17. 03 A	
ATOM		LE 751	64. 704 46. 632 42. 604 1. 00 15. 90 A	
ATOM		LE 751	64. 206 47. 849 41. 805 1. 00 17. 60 A	
ATOM ATOM	5839 CG2 II 5840 CG1 II		62. 893 47. 504 41. 088 1. 00 16. 17 A	
ATOM	5841 CD1 II		64. 065 49. 058 42. 736 1. 00 15. 94 A 63. 684 50. 332 42. 017 1. 00 12. 51 A	
ATOM		LE 751	00 851 10 011 10 505	
ATOM		E 751	63. 751 46. 341 43. 767 1. 00 16. 09 A 64. 062 46. 632 44. 919 1. 00 16. 37 A	
ATOM	5844 N TY	/R 752	62. 596 45. 759 43. 480 1. 00 16. 32 A	
ATOM	5845 CA TY		61. 651 45. 449 44. 551 1. 00 16. 16 A	
ATOM ATOM	5846 CB TY		60. 323 44. 967 43. 968 1. 00 13. 79 A	C
ATOM	5847 CG TY 5848 CD1 TY		59. 443 46. 126 43. 593 1. 00 12. 59 A	
ATOM	5849 CE1 TY		58. 840 46. 899 44. 580 1. 00 11. 61 A 58. 102 48. 026 44. 258 1. 00 9. 67 A	
ATOM	5850 CD2 TY		58. 102 48. 026 44. 258 1. 00 9. 67 A 59. 279 46. 510 42. 260 1. 00 12. 75 A	
ATOM	5851 CE2 TY	R 752	58. 543 47. 644 41. 930 1. 00 10. 28 A	Č
ATOM	5852 CZ TY		57. 964 48. 395 42. 940 1. 00 9. 02 A	č
ATOM ATOM	5853 OH TY		57. 278 49. 542 42. 642 1. 00 12. 10 A	0
ATOM	5854 C TY 5855 O TY		62. 226 44. 429 45. 522 1. 00 16. 42 A	C
ATOM	5856 N TH		61. 927 44. 467 46. 719 1. 00 16. 42 A 63. 056 43. 526 45. 004 1. 00 15. 74 A	0
ATOM	5857 CA TH		CO 700 40 504 15 005	N C
ATOM	5858 CB TH	R 753	63.700 42.521 45.835 1.00 16.30 A 64.502 41.510 44.985 1.00 15.57 A	C
ATOM	5859 OG1 TH		63. 601 40. 677 44. 253 1. 00 15. 74 A	ő
ATOM	5860 CG2 TH		65. 385 40. 641 45. 870 1. 00 10. 01 A	Č
ATOM ATOM	5861 C TH 5862 O TH		64. 678 43. 240 46. 758 1. 00 18. 17 A	C
ATOM	5863 N HI		64. 788 42. 923 47. 941 1. 00 19. 02 A 65. 388 44. 215 46. 199 1. 00 18. 78 A	0
ATOM	5864 CA HI		66 969 44 979 49 959	N C
ATOM	5865 CB HI	_	67. 189 45. 857 46. 023 1. 00 18. 90 A	C
ATOM	5866 CG HIS		68. 449 46. 379 46. 644 1. 00 19. 62 A	č
ATOM	5867 CD2 HIS		68. 786 47. 619 47. 070 1. 00 18. 70 A	Č
ATOM ATOM	5868 ND1 HIS 5869 CE1 HIS		69. 539 45. 576 46. 904 1. 00 18. 44 A	N
ATOM	5870 NE2 HIS		70. 493 46. 298 47. 462 1. 00 17. 52 A 70. 062 47. 541 47. 574 1. 00 19. 51 A	C
ATOM	5871 C HIS		CT CC0 45 000 10 005	N
ATOM	5872 0 HIS		66. 088 45. 876 49. 158 1. 00 19. 38 A	C 0
ATOM	5873 N MET	755	64.589 46.502 47.615 1.00 18.83 A	N N
ATOM	5874 CA MET		63. 854 47. 342 48. 558 1. 00 19. 68 A	Ĉ
ATOM ATOM	5875 CB MET 5876 CG MET		62. 758 48. 136 47. 839 1. 00 16. 86 A	C
ATOM	5876 CG MET 5877 SD MET		63. 283 49. 173 46. 876 1. 00 16. 00 A 62. 016 50. 314 46. 309 1. 00 20. 78 A	C
ATOM	5878 CE MET		01 100 40 000	S
ATOM	5879 C MET		61. 100 49. 270 45. 200 1. 00 15. 61 A 63. 232 46. 506 49. 676 1. 00 20. 27 A	C
			FEAT TION BOLDS	•

			FIG. 4-122	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	5929 CD GLN 5930 OE1 GLN 5931 NE2 GLN 5932 C GLN 5933 O GLN 5934 N CYS 5935 CA CYS 5936 C CYS 5937 O CYS 5938 CB CYS 5939 SG CYS 5940 N PHE 5941 CA PHE 5942 CB PHE 5942 CB PHE 5943 CG PHE 5944 CD1 PHE 5945 CD2 PHE 5946 CE1 PHE 5947 CE2 PHE 5948 CZ PHE 5948 CZ PHE 5949 C PHE 5950 O PHE 5951 N SER 5954 OG SER 5955 C SER 5956 O SER 5957 N LEU 5961 CD1 LEU 5962 CD2 LEU 5963 C LEU 5964 O LEU 5966 CD PRO 5966 CD PRO 5967 CA PRO 5968 CB PRO 5969 CG PRO 5960 CG PRO 5960 CG PRO 5960 CG PRO 5961 CD1 LEU 5962 CD2 LEU 5961 CD1 LEU 5962 CD2 LEU 5963 C LEU 5964 O LEU 5965 N PRO 5966 CD PRO 5967 CA PRO 5968 CB PRO 5969 CG PRO 5970 C PRO 5971 O PRO 5971 O PRO 5972 OXT PRO	761 761 761 761 762	68. 759	A C A O N A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C A A C C C A A C C C A A C C C A A C C C A A C C C A A C C C A A C C C A A C C C A A C C C A A C C C A A C C C A A C C C A A C C C A A C C C A A C C C C A A C C C C A A C C C C A A C C C C A A C C C C A A C C C C A C C C C A C C C C C C C C C C C C C C C C C C C C
TER ATOM ATOM ATOM	5973 PRO 5974 CB ASP 5975 CG ASP 5976 OD1 ASP	766 38 38	95. 909 45. 132 76. 302 1. 00 32. 66 96. 954 46. 047 75. 698 1. 00 32. 61	A 0 A B C B C
ATOM	5977 OD2 ASP	38 38		B 0 B 0

				FIG. 4-123	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	5982 N 5983 C 5984 C	ASP ASP ASP ASP SER ASER SER SER SER ARG ARG ARG ARG ARG	38 38 38 39 39 39 39 39 40 40 40 40	94. 533 46. 724 77. 638 1. 00 31. 81 B 93. 521 46. 648 76. 938 1. 00 32. 54 B 94. 842 44. 428 78. 423 1. 00 32. 95 B 95. 507 45. 557 77. 717 1. 00 32. 06 B 94. 844 47. 807 78. 344 1. 00 31. 40 B 93. 974 48. 982 78. 372 1. 00 30. 28 B 94. 048 49. 652 79. 741 1. 00 31. 88 B 95. 362 50. 119 80. 003 1. 00 34. 53 B 94. 289 50. 017 77. 305 1. 00 29. 15 B 93. 615 51. 049 77. 220 1. 00 30. 29 B 95. 312 49. 755 76. 499 1. 00 26. 40 B 95. 685 50. 686 75. 442 1. 00 24. 29 B 97. 004 50. 257 74. 788 1. 00 23. 19 B 98. 228 50. 429 75. 670 1. 00 20. 84 B	C O N C N C C O C C C C C C C C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	5993 N 5994 C 5995 N	E ARG Z ARG H1 ARG H2 ARG ARG ARG LYS A LYS B LYS G LYS O LYS	40 40 40 40 40 40 41 41 41 41 41	99. 404 48. 479 74. 728 1. 00 21. 28 B 100. 260 47. 812 73. 963 1. 00 22. 73 B 101. 247 48. 461 73. 361 1. 00 22. 52 B 100. 134 46. 497 73. 806 1. 00 22. 23 B 94. 604 50. 757 74. 376 1. 00 23. 29 B 93. 881 49. 793 74. 150 1. 00 23. 24 B 94. 494 51. 907 73. 725 1. 00 23. 55 B 93. 518 52. 076 72. 658 1. 00 24. 31 B 93. 386 53. 556 72. 274 1. 00 25. 29 B 94. 699 54. 209 71. 827 1. 00 29. 38 B 94. 505 55. 663 71. 365 1. 00 28. 84 B	C N C N C O N C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	6005 NZ 6006 C 6007 O 6008 N 6009 CA 6010 CB 6011 OG	LYS LYS LYS THR THR	41 41 42 42 42 42 42 42 42 43 43	93. 307 54. 922 69. 251 1. 00 27. 49 B 94. 028 51. 294 71. 458 1. 00 24. 04 B 95. 231 51. 072 71. 324 1. 00 24. 69 B 93. 118 50. 859 70. 595 1. 00 23. 54 B 93. 518 50. 130 69. 399 1. 00 22. 29 B 92. 454 49. 083 68. 959 1. 00 22. 69 B 91. 257 49. 753 68. 540 1. 00 21. 91 B 92. 128 48. 129 70. 101 1. 00 20. 28 B 93. 641 51. 178 68. 304 1. 00 22. 33 B 93. 386 52. 363 68. 541 1. 00 23. 36 B 94. 045 50. 750 67. 116 1. 00 20. 55 B	C N C O N C C C C C O N
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	6017 CB 6018 CG 6019 CD 6020 CE 6021 CD	TYR TYR TYR 1 TYR 2 TYR 2 TYR 2 TYR TYR TYR TYR TYR TYR TYR	43 43 43 43 43 43 43 43 43 43	94. 158 51. 662 65. 986 1. 00 19. 19 B 95. 233 51. 153 65. 020 1. 00 20. 32 B 95. 516 52. 062 63. 853 1. 00 19. 92 B 94. 888 51. 863 62. 629 1. 00 22. 19 B 95. 133 52. 694 61. 546 1. 00 21. 23 B 96. 403 53. 126 63. 970 1. 00 21. 09 B 96. 655 53. 972 62. 891 1. 00 21. 69 B 96. 013 53. 742 61. 682 1. 00 22. 25 B 96. 247 54. 553 60. 600 1. 00 25. 44 B 92. 770 51. 631 65. 349 1. 00 18. 52 B 92. 396 50. 640 64. 725 1. 00 17. 41 B	C C C C C C C C C C

					FΙ	G. 4	-124			(Continued)
ATOM ATOM ATOM	6027 6028 6029	N CA CB	THR	44 44	92. 007 90. 633 89. 762	3 52.802 2 53.748	65.019	1.00 18.55	B B B	N C C
ATOM ATOM	6030 6031		2 THR	44	90. 195 89. 875	53.409	67.346		B B	0 C
ATOM ATOM	6032 6033	C 0	THR THR	44	90. 521 91. 511	53. 741			B B	C 0
ATOM ATOM	6034 6035	N Ca		45 45	89. 296 89. 026			1.00 19.06 1.00 18.74	B B	N C
ATOM ATOM	6036 6037	CB CG	LEU LEU	45 45	87. 570 87. 163	53.489	61.327	1.00 17.33 1.00 17.35	B B	C C
ATOM ATOM	6038 6039		1 LEU 2 LEU	45 45	88. 050 85. 698	53.417	58.873	1. 00 15. 87 1. 00 16. 27	B B	C C
ATOM ATOM	6040 6041	C 0	LEU LEU	45 45	89. 300 89. 827	55. 240	61.638	1.00 19.82 1.00 21.32	B B	C 0
ATOM ATOM	6042 6043	N CA	THR THR	46 46	88. 948 89. 156		62. 707 62. 760	1.00 19.07 1.00 20.55	B B	N C
ATOM ATOM	6044 6045	CB OG1		46 46	88. 550 87. 148	57.700	64. 038 64. 083	1.00 21.32 1.00 21.56	B B	C 0
ATOM ATOM	6046 6047	C	THR THR	46 46	88. 745 90. 634	57.749	64. 053 62. 694	1.00 20.61 1.00 21.16	B B	C C
ATOM ATOM ATOM	6048 6049 6050	O N	THR ASP	46 47	90. 999 91. 491	56.945	62. 092 63. 313	1.00 21.06 1.00 21.00	B B	O N
ATOM ATOM	6051 6052	CA CB CG	ASP ASP ASP	47 47	92. 910 93. 731	57. 253 56. 273	63. 262 64. 110	1.00 22.97 1.00 25.34	B B	C C
ATOM ATOM	6053 6054	0D1	ASP ASP	47 47 47	93. 365 93. 116 93. 339	56. 322 57. 430	65. 578 66. 105	1.00 27.23 1.00 26.32	B B	C 0
ATOM ATOM	6055 6056	C 0	ASP ASP	47 47	93. 357 94. 057	55. 244 57. 178 58. 065	66. 208 61. 810	1.00 31.41 1.00 22.85	B B	0 C
ATOM ATOM	6057 6058	N CA	TYR TYR	48 48	92. 951 93. 332	56. 124 55. 998	61. 320 61. 114 59. 720	1. 00 24. 15 1. 00 20. 92 1. 00 21. 40	B B	0 N
ATOM ATOM	6059 6060	CB CG	TYR TYR	48 48	92. 823 92. 867	54. 676 54. 612	59. 136 57. 624	1. 00 21. 40 1. 00 19. 45 1. 00 18. 60	B B B	C C C
ATOM ATOM	6061 6062	CD1 CE1	TYR TYR	48 48	94. 062 94. 098	54. 787 54. 734	56. 927 55. 531	1.00 18.00 1.00 16.57	B B	C C
ATOM ATOM	6063 6064	CE2	TYR TYR	48 48	91. 702 91. 726	54. 383 54. 329	56. 885 55. 489	1. 00 21. 30 1. 00 19. 50	B B	C C
ATOM ATOM	6065 6066	CZ OH	TYR TYR	48 48	92. 925 92. 942	54. 503 54. 434	54. 822 53. 452	1. 00 18. 43 1. 00 18. 40	B B	Č O
ATOM ATOM	6067 6068	C 0	TYR TYR	48 48	92. 795 93. 547	57. 170 57. 853	58. 899 58. 207	1.00 21.85 1.00 21.92	B B	C 0
ATOM ATOM	6069 6070	N CA	LEU LEU	49 49	91. 497 90. 885	57. 416 58. 485	58. 996 58. 223	1.00 23.08 1.00 26.78	B B	N C
ATOM ATOM	6071 6072 6073	CB CG	LEU LEU	49 49	89. 359 88. 688	58. 437 57. 157	58. 381 57. 872	1.00 28.14 1.00 28.75	B B	C
ATOM ATOM ATOM	6074 6075		LEU LEU LEU	49 49 49	87. 188 89. 094 91. 391	57. 305 56. 889 59. 886	57. 980 56. 420 58. 544	1. 00 28. 04 1. 00 28. 45 1. 00 28. 33	B B B	C C C

			FIC	3. 4 -	125			(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	6091 ND2 6092 C 6093 O 6094 N 6095 CA 6096 CB 6097 OG1 6098 CG2 6099 C 6100 O 6101 N 6102 CA 6103 CB 6104 CG 6105 CD1 6106 CE1 6107 CD2 6108 CE2 6109 CZ 6110 OH 6111 C 6112 O 6113 N 6114 CA 6115 CB 6116 CG 6117 CD 6118 NE 6116 CG 6117 CD 6118 NE 6119 CZ 6120 NH1 A 6121 NH2 A 6122 C 6123 O	THR 52 THR 52 THR 52 TYR 53 TY	91. 404 91. 818 92. 299 91. 668 90. 159 89. 649 88. 239 87. 310 93. 811 94. 325 94. 525 95. 978 96. 502 95. 964 96. 358 95. 047 96. 472 97. 474 95. 770 96. 152 97. 474 97. 622 98. 274 97. 622 98. 274 98. 141 99. 541 99. 632 98. 937 99. 433 98. 782 97. 768 97. 768 97. 107 97. 622 98. 981 100. 187 101. 024 101. 760 101. 718 100. 360 100. 364 99. 157 98. 812 99. 585 97. 697 103. 202 103. 934	61. 743 62. 710 62. 353 62. 113 61. 543 62. 622 60. 456 60. 456 60. 416 60. 828 61. 524 60. 587 59. 742 60. 058 60. 030 60. 259 60. 867 59. 298 58. 900 57. 446 57. 209 57. 761 57. 566 56. 255 56. 813 56. 609 57. 761 56. 255 56. 813 60. 168 60. 456 60. 45	57. 673 59. 784 60. 204 61. 543 61. 478 60. 420 59. 970 61. 113 60. 288 60. 577 60. 033 60. 074 59. 090 57. 689 56. 986 57. 277 61. 471 62. 486 63. 870 64. 854 64. 698 64. 698 64. 698 64. 934 64. 698 65. 268 66. 291 66. 291 66. 389 16. 328 16. 328 16. 328 16. 328 16. 328 16. 328 16. 389 17. 634 18. 826 19. 0498 19.	1. 00 28. 77 1. 00 30. 17 1. 00 30. 95 1. 00 31. 36 1. 00 34. 69 1. 00 36. 08 1. 00 37. 00 1. 00 31. 05 1. 00 32. 05 1. 00 30. 75 1. 00 31. 14 1. 00 33. 97 1. 00 37. 06 1. 00 39. 83 1. 00 40. 54 1. 00 29. 86 1. 00 27. 72 1. 00 26. 81 1. 00 27. 72 1. 00 26. 88 1. 00 27. 72 1. 00 26. 88 1. 00 27. 48 1. 00 27. 48 1. 00 24. 69 1. 00 24. 64 1. 00 24. 69 1. 00 24. 44 1. 00 24. 67 1. 00 24. 64 1. 00 25. 33 1. 00 27. 74 1. 00 26. 35 1. 00 27. 75 1. 00 26. 88 1. 00 27. 88 1. 00 27. 96 1. 00 24. 89 1. 00 30. 80 1. 00 30. 80 1. 00 42. 89 1. 00 42. 89 1. 00 42. 89 1. 00 48. 52 1. 00 27. 73 1. 00 26. 62 1. 00 25. 96	B B B B B B B B B B B B B B B B B B B	ONCCCCNCONCCONCCCCNCNNCONCCCCNCNNCONCCCCNCNNCONCCCCNCNNCONCCCCNCNNCONCCCCCNCNNCONCCONCNNCONCCONCNNCONCCONCNNCONNCONCCONCNNCONCCONCNNCONNCONCCONCNNCONNCONCO
					-			

			1	FIG. 4-126	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	6160	CB LEU CG LEU	55555555555555555555555555555555555555	104. 959 58. 926 59. 515 1. 00 24. 45 B 105. 025 57. 911 58. 382 1. 00 22. 51 B 104. 335 56. 575 58. 631 1. 00 23. 77 B 104. 287 55. 792 57. 336 1. 00 23. 51 B 105. 083 55. 796 59. 703 1. 00 22. 83 B 105. 773 60. 161 59. 135 1. 00 24. 19 B 105. 428 60. 867 58. 187 1. 00 23. 47 B 106. 824 60. 456 59. 886 1. 00 23. 25 B 107. 631 61. 603 59. 532 1. 00 23. 25 B 107. 850 62. 028 60. 680 1. 00 25. 76 B 107. 850 62. 922 61. 697 1. 00 29. 15 B 108. 868 63. 560 62. 638 1. 00 31. 22 B 108. 225 64. 593 63. 548 1. 00 32. 59 B 109. 235 65. 233 64. 439 1. 00 34. 54 B 108. 818 61. 196 58. 330 1. 00 23. 24 B 109.	
ATOM ATOM	6162 6163	CA SER CB SER	59 59	112.085 64.604 52.909 1.00 21.33 B 112.245 64.839 51.479 1.00 22.11 B 110.920 65.275 50.852 1.00 21.08 B	N C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	6164 6165 6166 6167 6168 6169 6170 6171 6172	OG SER C SER O SER N LEU CA LEU CB LEU CG LEU CD1 LEU CD2 LEU C LEU	59 59 59 60 60 60 60 60	109. 985 64. 212 50. 843 1. 00 24. 94 B 113. 293 65. 895 51. 191 1. 00 21. 64 B 113. 099 67. 064 51. 491 1. 00 23. 87 B 114. 404 65. 485 50. 602 1. 00 21. 76 B 115. 449 66. 436 50. 273 1. 00 23. 50 B 116. 752 66. 062 50. 986 1. 00 22. 27 B 117. 406 64. 737 50. 612 1. 00 18. 62 B 118. 176 64. 900 49. 320 1. 00 17. 05 B 118. 338 64. 313 51. 724 1. 00 19. 95 B 115. 656 66. 478 48. 762 1. 00 24. 93 B	C O O N C C C C C

					FIG. 4-127	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	6175 6176 6177 6178 6180 6181 6182 6183 6184 6185 6186 6187 6188 6189 6190 6191 6192 6193 6194 6195 6196 6197 6198 6199 6200 6201 6202 6203 6204 6205 6206 6207 6212 6213 6214 6215 6215	CNE CON A CC C	ARG ARG ARG TRP	60 61 61 61 61 61 61 61 61 61 62 62 62 62 62 62 62 62 63 63 63 64 64 64 64 64 64 64 64 64 65 65 65 65 65 65 65 65 65 65 65 65 65	115. 176 65. 604 48. 029 1. 00 23. 79 B 116. 375 67. 495 48. 302 1. 00 26. 02 B 116. 634 67. 659 46. 881 1. 00 27. 11 B 115. 693 68. 728 46. 329 1. 00 32. 13 B 115. 779 68. 979 44. 833 1. 00 38. 27 B 115. 902 70. 243 44. 495 1. 00 41. 78 B 114. 937 70. 506 43. 063 1. 00 46. 51 B 114. 937 70. 506 43. 063 1. 00 49. 47 B 113. 671 72. 420 43. 307 1. 00 48. 74 B 113. 671 72. 420 43. 307 1. 00 48. 74 B 118. 800 68. 075 46. 676 1. 00 26. 01 B 118. 475 69. 180 47. 052 1. 00 26. 36 B 118. 877 67. 186 46. 095 1. 00 25. 15 B 120. 282 67. 488 45. 846 1. 00 24. 48 B 121. 095 66. 244 45. 355 1. 00 18. 16 B 121.	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	6216 C 6217 C 6218 O	A AB AG AD1 AD2 A	ISP ISP ISP ISP		127. 306 66. 947 44. 728 1. 00 32. 55 B 128. 576 66. 633 43. 945 1. 00 33. 28 B 129. 158 65. 286 44. 302 1. 00 35. 12 B 128. 446 64. 261 44. 158 1. 00 33. 02 B 130. 331 65. 259 44. 728 1. 00 37. 02 B 127. 636 67. 045 46. 211 1. 00 32. 66 B 128. 076 66. 069 46. 818 1. 00 31. 78 B	C C C O C C
	II	11		UU	127. 399 68. 217 46. 796 1. 00 33. 06 B	N

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				FIG.	4 - 128	8		(Continued)					
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	6223 6224 6225 6226 6227 6228 6229 6231 6232 6233 6234 6235 6236 6237 6238 6240 6241 6242 6243 6244 6245 6246 6247 6248 6251 6252 6253 6253 6253 6253 6253 6253 6253	CA HIS CB HIS CCB HIS CCD2 HIS CD2 HIS CD2 HIS CD1 HIS CE1 HIS CE1 HIS CE2 HIS CCB GLU CCB TYR CCB LEU CCB LEU CCB LEU CCB LEU CCB LEU CCB TYR	666 666 666 666 667 677 677 677 677 677	127. 704 68 128. 892 69 130. 032 69 131. 260 68 129. 959 69 131. 092 68 131. 897 68 136. 547 69 126. 602 69 125. 505 69 124. 379 70 124. 457 71 125. 601 72 125. 745 73 126. 408 74 125. 207 74 123. 015 69 122. 872 69 122. 012 69 120. 347 68 120. 347 68 120. 347 68 120. 347 68 120. 347 68 120. 347 68 120. 347 68 120. 373 67 119. 339 68 119. 312 68 121. 391 67 121. 379 66 120. 333 67 120. 300 66 119. 657 70 119. 961 71 118. 497 70 117. 492 71 116. 729 72 117. 545 73 116. 729 72 117. 545 73 116. 508 70 119. 961 71 118. 497 70 117. 492 71 116. 729 72 117. 545 73 116. 508 70 119. 961 71 118. 497 70 117. 492 71 116. 729 72 117. 545 73 116. 729 72 117. 545 73 116. 508 70 119. 961 71 118. 497 70 114. 492 71 116. 729 72 117. 545 73 116. 508 70 117. 492 71 116. 508 70 117. 492 71 116. 508 70 117. 492 71 116. 508 70 117. 492 71 116. 508 70 117. 545 73 116. 508 70 117. 545 73 116. 508 70 117. 492 71 116. 729 72 117. 545 73 116. 508 70 117. 492 71 116. 508 70 117. 492 71 117. 545 73 116. 508 70 117. 545 73 116. 508 70 117. 545 73 116. 508 70 117. 545 73 116. 508 70 117. 545 73 117. 545 73 117. 545 73 116. 508 70 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 545 73 117. 5	4 - 1 2 8 8. 440	3 1.00 32.64 9 1.00 35.63 6 1.00 39.09 9 1.00 40.29 7 1.00 41.80 8 1.00 42.37 1.00 42.11 1.00 31.01 1.00 30.92 1.00 30.05 1.00 28.07 1.00 29.99 1.00 32.09 1.00 32.09 1.00 32.09 1.00 32.09 1.00 32.09 1.00 27.52 1.00 27.52 1.00 27.52 1.00 27.52 1.00 27.52 1.00 27.52 1.00 27.52 1.00 27.52 1.00 27.52 1.00 27.52 1.00 27.52 1.00 27.52 1.00 27.52 1.00 27.52 1.00 27.52 1.00 27.52 1.00 27.52 1.00 27.52 1.00 27.52 1.00 27.89 1.00 26.72 1.00 26.72 1.00 27.89 1.00 24.29 1.00 23.81 1.00 19.95	888888888888888888888888888888888888888	$\tt CCCCNCNCONCCCCOOCONCCCCCCCONCCCCCONCCCCCC$					
ATOM ATOM	6265 6266	CG TYR CD1 TYR CE1 TYR	70 70 70 70 70 70 70 70	114. 910 69. 114. 396 68. 113. 544 67. 114. 553 69. 113. 701 69. 113. 199 67. 112. 346 67. 114. 056 71.	348 54. 592 114 54. 206 398 55. 038 847 55. 842 141 56. 686 918 56. 276 221 57. 103 796 52. 983	1. 00 26. 47 1. 00 25. 75 1. 00 26. 40 1. 00 28. 33 1. 00 28. 03 1. 00 28. 21 1. 00 30. 20 1. 00 34. 45	B B B	C C					
			•		SUBSTITUTE SHEET (RULE 26)								

	FIG. 4-129	(Continued)
ATOM 6272 O TYR ATOM 6273 N LYS ATOM 6274 CA LYS ATOM 6275 CB LYS ATOM 6276 CG LYS ATOM 6277 CD LYS ATOM 6277 CD LYS ATOM 6278 CE LYS ATOM 6279 NZ LYS ATOM 6280 C LYS ATOM 6281 O LYS ATOM 6282 N GLN ATOM 6283 CA GLN ATOM 6283 CA GLN ATOM 6284 CB GLN ATOM 6285 CG GLN ATOM 6286 CD GLN ATOM 6287 OE1 GLN ATOM 6288 NE2 GLN ATOM 6288 NE2 GLN ATOM 6289 C GLN ATOM 6290 O GLN ATOM 6291 N GLU ATOM 6292 CA GLU ATOM 6292 CA GLU ATOM 6293 CB GLU ATOM 6293 CB GLU ATOM 6294 CG GLU ATOM 6295 CD GLU ATOM 6296 OE1 GLU ATOM 6297 OE2 GLU ATOM 6298 C GLU ATOM 6299 O GLU ATOM 6299 O GLU ATOM 6290 O GLU ATOM 6291 CA ASN ATOM 6301 CA ASN ATOM 6302 CB ASN ATOM 6303 CG ASN ATOM 6304 OD1 ASN ATOM 6305 ND2 ASN ATOM 6306 C ASN ATOM 6307 O ASN ATOM 6307 O ASN ATOM 6308 N ASN ATOM 6307 O ASN ATOM 6309 CA ASN ATOM 6309 CA ASN ATOM 6309 CA ASN ATOM 6301 CB ASN ATOM 6301 CB ASN ATOM 6311 CG ASN ATOM 6311 CG ASN ATOM 6311 CG ASN ATOM 6312 OD1 ASN ATOM 6313 ND2 ASN ATOM 6314 C ASN ATOM 6315 O ASN ATOM 6315 O ASN ATOM 6316 N ILE ATOM 6317 CA ILE ATOM 6317 CA ILE ATOM 6317 CA ILE	70 114. 425 72. 914 53. 336 1. 71 112. 787 71. 410 53. 002 1. 71 111. 714 72. 284 53. 461 1. 71 110. 408 71. 904 52. 763 1. 71 109. 994 72. 828 51. 640 1. 71 109. 416 74. 116 52. 192 1. 71 108. 213 73. 827 53. 075 1. 71 107. 193 73. 012 52. 354 1. 71 107. 193 73. 012 52. 354 1. 71 110. 789 71. 323 55. 457 1. 71 110. 789 71. 323 55. 457 1. 72 112. 192 73. 055 55. 723 1. 72 113. 145 73. 853 57. 851 1. 72 113. 145 73. 853 57. 851 1. 72 113. 582 72. 412 59. 895 1. <t< td=""><td>00 33. 43</td></t<>	00 33. 43
	76 112.883 77.343 53.077 1.00 76 113.837 76.424 52.483 1.00 76 113.871 76.616 50.962 1.00 76 114.705 75.524 50.310 1.00) 45. 23 B N

				FIC	G. 4-	1 3 0			(Continued)
ATOM 632 ATOM 632	2 C	ILE ILE	76 76	112. 341 115. 243	77.009 76.589	48. 967 53. 043	1.00 42.01 1.00 39.85	B B	C C
ATOM 632	1 N	ILE LEU		115. 758 115. 862	77. 701 75. 472	53. 150 53. 400	1.00 41.15 1.00 36.42	B B	O N
ATOM 632 ATOM 632		LEU LEU		117. 208 117. 227	75. 498 74. 901	53. 941 55. 351	1.00 34.22 1.00 34.28	B B	C C
ATOM 632 ATOM 632		LEU LEU	77 77	116. 155 116. 435	75. 359 74. 728	56. 346 57. 701	1.00 34.54 1.00 33.23	B B	C C
ATOM 632	CD2	LEU	77	116.149	76.874	56.460	1.00 34.45	В	C
ATOM 633 ATOM 633		LEU LEU	77 77	118. 121 117. 657	74. 683 73. 821	53. 036 52. 289	1.00 32.91 1.00 32.49	B B	C 0
ATOM 633	2 N	VAL	78	119.417	74.967	53. 103	1.00 30.72	В	N
ATOM 633: ATOM 633:		VAL VAL	78 78	120. 409 121. 227	74. 253 75. 227	52. 308 51. 431	1.00 29.87 1.00 30.20	В В	C C
ATOM 633 ATOM 633		VAL VAL	78	122.327	74.480	50.691	1.00 29.01 1.00 31.37	В	C
ATOM 633		VAL	78 78	120. 311 121. 346	75. 906 73. 523	50. 448 53. 263	1.00 31.37	В В	C C
ATOM 6333 ATOM 6333		VAL PHE	78 79	121. 781 121. 660	74. 087 72. 272	54. 261 52. 956	1.00 28.38 1.00 26.51	B B	0 N
ATOM 634) CA	PHE	79	122.530	71.496	53.821	1.00 24.85	В	C
ATOM 634 ATOM 634		PHE PHE	79 79	121.807 120.680	70. 247 70. 531	54. 338 55. 296	1.00 24.45 1.00 22.62	В	C C
ATOM 6343	CD1	PHE	79	119.499	71.120	54.857	1.00 20.15	В	C
ATOM 6344 ATOM 6344		PHE PHE	79 79	120. 789 118. 448	70. 168 71. 338	56. 636 55. 733	1.00 19.84 1.00 20.35	B B	C C
ATOM 6346 ATOM 6346	CE2	PHE	79	119.749	70.382	57. 513	1.00 16.96	В	C
ATOM 6348		PHE PHE	79 79	118. 573 123. 815	70. 967 71. 036	57. 065 53. 151	1.00 18.97 1.00 24.95	B B	C
ATOM 6349 ATOM 6350		PHE ASN	79 80	123. 841 124. 876	70. 729 70. 992	51.960	1.00 24.94	В	0 .
ATOM 635	CA	ASN	80	126.174	70.518	53. 948 53. 517	1.00 23.66 1.00 23.32	B B	N C
ATOM 6353 ATOM 6353		ASN ASN	80 80	127. 276 128. 653	71.307 70.689	54. 220 54. 032	1.00 22.91 1.00 22.91	B B	C
ATOM 6354	0D1	ASN	80	128.916	69.567	54.486	1.00 23.26	В	0
ATOM 6350 ATOM 6350		ASN ASN	80 80	129. 542 126. 156	71.421 69.077	53. 364 54. 018	1.00 21.99 1.00 24.17	B B	N C
ATOM 6357	0	ASN	80	126.168	68.842	55. 222	1.00 25.80	В	0
ATOM 6358 ATOM 6359		ALA ALA	81 81	126. 116 126. 054	68. 116 66. 713	53. 105 53. 496	1.00 23.17 1.00 24.07	B B	N C
ATOM 6360 ATOM 6361		ALA ALA	81 81	126. 025 127. 167	65.819 66.256	52. 246 54. 434	1.00 20.69 1.00 25.23	B B	C C
ATOM 6362	0	ALA	81	126.925	65.462	55.347	1.00 25.26	В	0
ATOM 6363 ATOM 6364		GLU GLU	82 82	128. 377 129. 525	66. 764 66. 351	54. 222 55. 024	1.00 26.73 1.00 29.51	B B	N C
ATOM 6365	CB	GLU	82	130.820	66.835	54.361	1.00 32.02	В	C
ATOM 6366 ATOM 6367		GLU GLU	82 82	132. 124 132. 287	66. 326 64. 800	55. 005 54. 955	1.00 35.72 1.00 38.90	B B	C C
ATOM 6368 ATOM 6369	0E1	GLU GLU	82 82	132.064 132.659	64. 191 64. 209	53. 884 55. 995	1.00 38.71 1.00 40.81	B B	0

										(0): 1)
					FIC	3. 4 -	131			(Continued)
ATOM	6370	С	GLU	82	129. 528	66. 757	56. 497	1.00 29.17	В	С
ATOM	6371	ŏ	GLU	82	130. 102	66.051	57. 324		В	0
ATOM	6372		TYR	83	128. 888	67. 872	56.834		В	N N
ATOM	6373			83	128. 877	68. 329	58. 223	1.00 28.95	В	C
ATOM	6374			83	129.504	69. 722	58. 320		В	Č
ATOM	6375	CG		83	130. 821	69. 834	57. 596	1.00 33.40	В	C
ATOM	6376		1 TYR	83	131. 914	69.049	57. 963	1.00 33.40	В	C
ATOM	6377		1 TYR	83	133. 120	69. 129	57. 271	1.00 36.07	В	Č
ATOM	6378		2 TYR	83	130. 966	70. 704	56.517	1.00 35.97	В	Č
ATOM	6379		2 TYR	83	132. 162	70. 791	55.815	1.00 36.91	В	č
ATOM	6380	CZ		83	133. 234	70.003	56. 195	1.00 38.12	В	Č
ATOM	6381	OH		83	134. 413	70.091	55. 486	1.00 42.42	В	Ö
ATOM	6382	C	TYR	83	127. 490	68. 355	58. 853	1.00 28.16	В	Č
ATOM	6383	Ŏ	TYR	83	127. 340	68. 093	60.044	1.00 29.04	В	Ö
ATOM	6384	Ň	GLY	84	126. 478	68. 684	58. 063	1.00 25.68	В	N
ATOM	6385	CA	GLY	84	125. 136	68. 726	58. 601		В	Č
ATOM	6386	C	GLY	84	124.668	70. 137	58. 880	1.00 24.95	В	č
ATOM	6387	0	GLY	84	123. 511	70. 345	59. 222	1.00 23.68	B	ŏ
ATOM	6388	N	ASN	85	125.565	71.109	58. 745	1.00 26.40	В	N
ATOM	6389	CA	ASN	85	125. 201	72. 501	58. 984	1.00 27.79	В	C
ATOM	6390	CB	ASN	85	126.446	73. 366	59. 181	1.00 28.01	B	č
ATOM	6391	CG	ASN	85	127.356	73. 363	57. 975	1.00 31.32	B	č
ATOM	6392	0D1	ASN	85	128.051	72. 384	57.697	1.00 31.73	B	ŏ
ATOM	6393		2 ASN	85	127.338	74.472	57. 250	1.00 33.71	B	Ň
ATOM	6394	C	ASN	85	124.381	73.023	57.813	1.00 28.62	B	Ċ
ATOM	6395	0	ASN	85	124. 432	72.472	56.720	1.00 28.74	B	Ö
ATOM	6396	N	SER	86	123.622	74.085	58.043	1.00 30.17	B	N
ATOM	6397	CA	SER	86	122.787	74.633	56.991	1.00 32.38	B	Ĉ
ATOM	6398	CB	SER	86	121.392	74.005	57.061	1.00 31.71	В	- Č
ATOM	6399	0G	SER	86	120. 734	74.380	58. 256	1.00 32.32	В	0
ATOM	6400	C	SER	86	122.658	76. 145	57.063	1.00 33.63	В	Ċ
ATOM	6401	0	SER	86	123. 307	76.800	57.874	1.00 34.72	В	0
ATOM	6402	N	SER	87	121.806	76.682	56. 195	1.00 35.45	В	N
ATOM	6403	CA	SER	87	121.530	78. 111	56.115	1.00 35.95	В	С
ATOM	6404	CB	SER	87	122.588	78. 825	55.280	1.00 35.50	В	С
ATOM	6405	0G	SER	87	123. 887	78. 635	55.810	1.00 39.27	В	0
ATOM	6406	C	SER	87	120. 191	78. 233	55.418	1.00 36.74	В	С
ATOM	6407	0.	SER	87	119.832	77. 369	54.625	1.00 38.47	В	0
ATOM	6408	N	VAL	88		79. 288	55. 723	1.00 37.17	В	N
ATOM	6409	CA	VAL	88		79. 498	55. 084	1.00 36.32	В	C
ATOM	6410	CB	VAL	88		80. 636	55. 750	1.00 37.21	В	С
ATOM	6411		VAL	88		80.916	54.954	1.00 36.84	В	C C
ATOM	6412		VAL	88		80. 260	57. 186	1.00 38.04	В	С
ATOM	6413	C	VAL	88		79. 897	53. 647	1.00 36.83	В	C
ATOM	6414	0	VAL	88		80. 782	53. 379	1.00 36.34	В	0
ATOM	6415	N	PHE	89		79. 240	52. 719	1.00 36.53	В	N
ATOM	6416	CA	PHE	89		79. 552	51. 314	1.00 37.05	В	C
ATOM	6417	CB	PHE	89		78. 262	50. 491	1.00 34.62	В	C C
ATOM	6418	CG	PHE	89		78. 474	49.014	1.00 31.67	В	C
				SU	JBSTITUTE	SHEET (RULE 26)		
						•				

	FIG. 4-132	(Continued)
ATOM 6459 CB THR ATOM 6460 OG1 THR ATOM 6461 CG2 THR ATOM 6462 C THR ATOM 6463 O THR ATOM 6464 N PHE ATOM 6465 CA PHE ATOM 6466 CB PHE	## F I G. 4 - 1 3 2 ## 116.963	B C C C C C C C C C C C C C C C C C C C
		-

										(Continued)
					FIG	3.4·	- 133			(Continuou)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	6468 6469 6470 6471 6472 6473 6474 6475	CD: CE: CZ: CZ: CO: N: CA	PHE PHE PHE PHE PHE PHE ASP	95 95 95 95 95 96 96	107. 978 107. 476 109. 095 108. 594 109. 403 104. 825 103. 740 104. 941 103. 775	83. 326 85. 290 83. 091 85. 061 83. 960 86. 105 85. 784 86. 681 86. 964	48. 268 47. 005 47. 473 46. 205 46. 441 50. 639 50. 149 51. 835 52. 668	1.00 51.86 1.00 51.89 1.00 50.37 1.00 51.43 1.00 50.62 1.00 55.66 1.00 55.16 1.00 56.69 1.00 57.24	B B B B B B	C C C C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	6477 6478 6479 6480 6481 6482 6483 6484 6485		ASP ASP ASP ASP ASP GLU GLU GLU GLU	96 96 96 96 96 97 97 97	104. 167 104. 793 104. 234 105. 835 102. 674 101. 498 103. 050 102. 068 102. 389 102. 397	87. 785 86. 945 85. 875 87. 366 87. 712 87. 401 88. 703 89. 496 90. 994 91. 553		1.00 58.96 1.00 60.91 1.00 60.82 1.00 62.59 1.00 57.24 1.00 58.26 1.00 57.07 1.00 57.68 1.00 59.15 1.00 61.76	B B B B B B	C C O C O N C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	6487 6488 6489 6490 6491 6492 6493 6494 6495	CD OE1	GLU GLU GLU GLU PHE PHE PHE	97 97 97 97 97 98 98 98	103. 629 103. 714 104. 514 101. 970 101. 652 102. 234 102. 181 102. 730 102. 792	91. 140 91. 490 90. 467 89. 123 89. 972 87. 859 87. 393 85. 965	52. 729 53. 927 52. 155 48. 917 48. 080 48. 598 47. 214 47. 117	1.00 63.57 1.00 63.88 1.00 64.73 1.00 56.86 1.00 58.05 1.00 54.75 1.00 52.58 1.00 52.58	B B B B B B	C O O C O N C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	6496 6497 6498 6499 6500 6501 6502 6503	CD1 CD2 CE1 CE2 CZ C O N	PHE PHE PHE PHE PHE PHE PHE PHE	98 98 98 98 98 98 98	103. 564 102. 064 103. 609 102. 103 102. 876 100. 764 100. 578 99. 770	85. 434 86. 073 84. 305 85. 597 83. 822 84. 469 87. 448 87. 544 87. 383	45. 713 44. 749 45. 348 43. 445 44. 044 43. 092 46. 641 45. 427 47. 523	1.00 51.74 1.00 50.75 1.00 51.54 1.00 50.51 1.00 50.40 1.00 49.83 1.00 51.24 1.00 50.42 1.00 50.67	B B B B B B	C C C C C C N
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	6508 6509 6510 6511 6512 6513 6514	CD2 ND1 CE1 NE2	HIS HIS	99 99 100 100 100 100 100 100 100 100	98. 383 97. 918 97. 020 98. 530 98. 200 98. 787 98. 004 98. 345 96. 711 96. 288 97. 262 98. 822	87. 441 86. 192 86. 246 85. 065 83. 780 83. 686 84. 414 85. 437 84. 075 84. 857 85. 691 82. 677	47. 094 46. 376 45. 540 46. 712 46. 104 44. 694 43. 651 42. 833 43. 321 42. 344 42. 029 46. 940	1.00 48.74 1.00 47.41 1.00 48.42 1.00 45.49 1.00 43.24 1.00 41.93 1.00 39.37 1.00 38.83 1.00 39.65 1.00 38.71 1.00 42.56	B B B B B B B B B B	C C O N C C C C N C

F I G. 4 - 1 3 5 (Continued)

ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	CBCGCCDCONCACBCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	LEELEER RESEARCE OF PROPERTY OF STATES OF STAT	107 107 107 107 107 107 107 108 108 108 108 109 109 109 109 110 110 110 110 110 111 111	115. 634 116. 885 115. 050 114. 056 115. 315 115. 418 116. 534 116. 936 117. 789 117. 789 118. 223 118. 394 118. 003	76. 576 77. 328 77. 161 76. 271 76. 305 77. 102 78. 439 79. 144 76. 347 76. 484 75. 554 74. 172 73. 983 75. 619 75. 139 76. 847 77. 691 78. 689 79. 543 79. 548 79.	43. 354 42. 987 44. 639 45. 321 40. 901 40. 548 40. 187 38. 959 38. 350 39. 245 39. 403 40. 546 38. 869 37. 547 36. 836 39. 499 40. 403 39. 562 38. 504 37. 960 38. 730 36. 767	4 1.00 21.79 7 1.00 21.05 8 1.00 21.30 1.00 23.96 1.00 25.00 8 1.00 27.32 1.00 24.67 1.00 24.23 1.00 23.85 1.00 23.56 1.00 25.01 1.00 25.28 1.00 25.25 1.00 25.10 1.00 26.01	8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8	CCCCCCONCCOCONCCCCCONCCCONCCCCONCONCCCCCC
		CBCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	CB ILE CG2 ILE CG3 ILE CG4 ILE CG5 ILE CG6 ILE CG6 ILE CG7 ILE CG7 ILE CG8 ILE CG8 ILE CG9 ILE	CB ILE 107 CG1 ILE 107 CG1 ILE 107 CD1 ILE 107 C ILE 107	CB ILE 107 115.63 CG2 ILE 107 116.88 CG1 ILE 107 115.050 CD1 ILE 107 115.315 C ILE 107 115.315 C ILE 107 115.418 N SER 108 115.788 CA SER 108 116.534 CB SER 108 116.936 CG SER 108 117.786 C SER 108 117.786 C SER 108 117.789 O SER 108 118.223 N PRO 109 118.394 CD PRO 109 118.003 CA PRO 109 118.003 CA PRO 109 120.023 CG PRO 109 120.726 O PRO 109 120.726 O PRO 109 121.413 N ASP 110 120.923 CA ASP 110 121.988 CB ASP 110 121.988 CB ASP 110 121.342 OD1 ASP 110 122.465 CG ASP 110 121.391 C ASP 110 121.391 C ASP 110 122.379 N GLY 111 120.397 CA GLY 111 119.663 O GLY 111 119.663 O GLY 111 119.665 CA GLY 111 119.673 O GLY 111 119.665 CA GLN 112 119.460 CB GLN 112 120.095 CG GLN 112 120.0885 CD GLN 112 120.0885 CD GLN 112 120.085 CD GLN 112 120.0885 CD GLN 112 120.095 CG GLN 112 120.09	CB ILE 107 115.634 76.576 CG2 ILE 107 116.885 77.328 CG1 ILE 107 115.050 77.161 CD1 ILE 107 115.050 77.161 CD1 ILE 107 115.315 76.305 CO ILE 107 115.315 76.305 CO ILE 107 115.418 75.132 N SER 108 116.534 77.102 CB SER 108 116.534 77.102 CB SER 108 116.936 78.439 OG SER 108 117.786 79.144 C SER 108 117.789 76.347 O SER 108 117.789 76.347 O SER 108 117.789 76.347 O SER 108 117.789 76.347 CD PRO 109 118.394 75.554 CD PRO 109 118.003 75.282 CA PRO 109 118.003 75.282 CA PRO 109 120.023 74.172 CG PRO 109 120.023 74.172 CG PRO 109 120.023 74.172 CG PRO 109 120.023 76.847 CA ASP 110 120.923 76.847 CA ASP 110 120.923 76.847 CA ASP 110 121.398 77.691 CB ASP 110 121.392 79.543 OD1 ASP 110 121.391 79.912 C ASP 110 121.391 79.912 C ASP 110 121.391 79.912 C ASP 110 122.379 79.248 N GLY 111 120.397 78.197 CA GLY 111 119.945 78.863 C GLY 111 119.945 78.863	CB ILE 107	CB ILE 107	CB ILE 107

				•						
					FΙ	G. 4	- 136	}		(Continued)
ATOM ATOM	6615 6616		PHE PHE		117. 386 114. 831				B B	C C
ATOM	6617		PHE		115. 308	79.829			B	Ö
ATOM	6618		ILE		113. 557				В	N
MOTA	6619				112.630	80. 258			В	C
ATOM ATOM	6620 6621		ILE 2 ILE		112. 394	80.504			В	C
ATOM	6622		I ILE		111. 911 111. 378	81.915 79.490			В	C
ATOM	6623		1 ILE		111. 336	79. 490			B B	C C
ATOM	6624		ILE		111. 336	80.403			В	Č
ATOM	6625	Õ	ILE		110. 895	81.508			В	0
ATOM	6626	N	LEU		110.756			1.00 30.43	В	Ň
ATOM	6627	CA			109.516				B	Ċ
ATOM	6628	CB	LEU		109. 596				В	Ċ
ATOM	6629	CG			108. 449	77.898		1.00 28.22	В	C
ATOM	6630		LEU		108. 425			1.00 28.47	В	C
ATOM ATOM	6631 6632	CD?	2 LEU		108. 645			1.00 29.52	В	Č
ATOM	6633	0	LEU LEU		108. 424			1.00 29.59	В	C
ATOM	6634	N	LEU		108. 370 107. 568			1.00 30.72	В	0
ATOM	6635	CA	LEU		106.479			1.00 30.29 1.00 30.17	B B	N C
ATOM	6636	CB	LEU	116	106. 129			1.00 30.17	В	C C
ATOM	6637	CG	LEU	116	107. 277		43. 544	1.00 33.66	В	C
ATOM	6638		LEU	116	106.732			1.00 33.41	В	Č
ATOM	6639		LEU	116	107. 957	80.821	44. 552	1.00 34.07	B	Č
ATOM	6640	C	LEU	116	105. 270	79. 215		1.00 30.44	В	C
ATOM	6641	0	LEU	116	104. 835	79.845		1.00 30.69	В	0
ATOM ATOM	6642	N	GLU	117	104. 724	78. 091	41.804	1.00 30.37	В	N
ATOM	6643 6644	CA CB	GLU GLU	117	103. 563	77.513		1.00 29.50	В	C
ATOM	6645	CG	GLU	117 117	103. 813 102. 671	76.017 75.210		1.00 30.63	В	C
ATOM	6646	CD	GLU	117	102. 071	73. 728	40. 368 40. 270	1.00 32.07 1.00 33.58	В	C
ATOM	6647		GLU	117	103. 772	73. 341	39. 340	1.00 33.58	B B	C 0
ATOM	6648		GLU	117	102.566			1.00 32.35	В	0
ATOM	6649	C	GLU	117	102.312	77. 756	42.009	1.00 29.67	B	C
ATOM	6650	0	GLU	117	102.333	77.583	43. 228	1.00 27.89	B.	ŏ
ATOM	6651	N	TYR	118	101. 235	78. 184	41.355	1.00 29.27	B	N
ATOM	6652	CA	TYR	118	99. 966	78. 423	42.026	1.00 28.00	В	Ċ
ATOM	6653	CB	TYR	118	99. 928	79.818	42.643	1.00 29.37	В	C
ATOM ATOM	6654 6655	CG	TYR	118	100.036	80.955	41.659	1.00 29.69	В	C .
ATOM	6656		TYR TYR	118	101.256	81.301	41.092	1.00 30.04	В	C
ATOM	6657		TYR	118 118	101. 355 98. 915	82.373 81.703	40. 210 41. 316	1.00 31.36	В	C
ATOM	6658		TYR	118	99.003	82. 768	40. 439	1.00 30.41 1.00 31.17	В	C
ATOM	6659	CZ	TYR	118	100. 222	83. 101	39. 891	1.00 31.17	B B	C C
ATOM	6660	ОH	TYR	118	100. 298	84. 179	39. 039	1.00 31.30	В	0
ATOM	6661	C	TYR	118	98. 814	78. 240	41.038	1.00 27.66	В	C
ATOM	6662	0	TYR	118	99.046	77.917	39. 874	1.00 26.73	B	ŏ
ATOM	6663	N	ASN	119	97. 582	78.450	41.499	1.00 27.22	B	N

					(Continued)
				FIG. 4-137	(• • • • • • • • • • • • • • • • • • •
ATOM 66	68 ND 69 C 70 O 71 N 72 CA 73 CB 74 CG 75 CC 76 CE 77 CD 78 CZ 80 OH 81 C 82 O 83 CA 85 CG 88 CG	ASN ASN 1 ASN 2 ASN ASN ASN TYR TYR TYR	119 119 119 119 119 119 120 120 120 120 120 120 120 121 121 121	96. 397 78. 261 40. 659 1. 00 27. 10 B 96. 422 79. 203 39. 449 1. 00 27. 22 B 95. 918 80. 599 39. 777 1. 00 27. 62 B 94. 905 80. 761 40. 456 1. 00 26. 76 B 96. 613 81. 612 39. 277 1. 00 25. 87 B 96. 342 76. 810 40. 171 1. 00 27. 88 B 95. 923 76. 534 39. 045 1. 00 27. 93 B 96. 771 75. 888 41. 028 1. 00 27. 57 B 96. 795 74. 466 40. 702 1. 00 29. 01 B 97. 396 73. 669 41. 866 1. 00 30. 85 B 97. 421 72. 171 41. 635 1. 00 32. 83 B 98. 466 71. 568 40. 940 1. 00 33. 76 B 98. 484 70. 190 40. 717 1. 00 35. 03 B 96. 389 71. 358 42. 100 1. 00 34. 41 B 96. 394 69. 981 41. 880 1. 00 34. 35 B 97. 444 69. 403 41. 191 1. 00 35. 47 B 97. 462 68. 039 40. 987 1. 00 35. 56 B 95. 431 73. 863 40. 364 1. 00 29. 17 B 94. 458 74. 034 41. 099 1. 00 31. 09 B 95. 368 73. 148 39. 248 1. 00 27. 53 B 94. 136 72. 487 38. 842 1. 00 27. 53 B 94. 136 72. 487 38. 842 1. 00 25. 25 B 92. 105 72. 534 37. 376 1. 00 25. 23 B 92. 105 72. 534 37. 376 1. 00 25. 23 B 94. 124 70. 082 38. 977 1. 00 24. 18 B 94. 527 71. 130 38. 275 1. 00 24. 18 B 94. 124 70. 082 38. 977 1. 00 24. 18 B 94. 124 70. 082 38. 977 1. 00 24. 16 B 94. 464 68. 735 38. 570 1. 00 24. 24 B 94. 295 67. 780 39. 754 1. 00 23. 05 B 94. 510 66. 327 39. 390 1. 00 20. 04 B 94. 402 63. 950 40. 161 1. 00 20. 85 B 93. 692 68. 180 37. 387 1. 00 24. 10 B	(Continued) C C C C C C C C C C C C C C C C C C
ATOM 669 ATOM 669	08 O 09 N	LYS GLN	122 123	92. 516 68. 488 37. 189 1. 00 23. 23 B 94. 384 67. 368 36. 592 1. 00 23. 36 B	C O N
ATOM 670 ATOM 670 ATOM 670 ATOM 670	1 CB 12 CG	GLN GLN GLN	123 123 123	93. 758 66. 691 35. 472 1. 00 21. 22 B 94. 455 67. 007 34. 145 1. 00 20. 62 B 93. 689 66. 433 32. 948 1. 00 23. 42 B	C C C
ATOM 670 ATOM 670 ATOM 670 ATOM 670	04 OE1 05 NE2 06 C 07 O	GLN GLN GLN GLN GLN	123 123 123 123 123	94. 242 66. 857 31. 591 1. 00 24. 37 B 95. 399 66. 606 31. 275 1. 00 26. 71 B 93. 402 67. 493 30. 779 1. 00 23. 80 B 93. 856 65. 194 35. 805 1. 00 20. 06 B 93. 258 64. 741 36. 786 1. 00 17. 04 B	C O N C O
ATOM 670 ATOM 671 ATOM 671 ATOM 671 ATOM 671	9 CA 0 CB 1 CG	TRP TRP TRP TRP TRP	124 124 124 124 124	94. 630 64. 438 35. 030 1. 00 17. 49 B 94. 753 63. 009 35. 276 1. 00 16. 75 B 95. 165 62. 298 33. 984 1. 00 16. 19 B 94. 351 62. 735 32. 797 1. 00 18. 11 B 92. 939 63. 014 32. 764 1. 00 17. 55 B	N C C C

				with.	· F I (G. 4-	138			(Continued)
ATOM	6713	CE2	TRP	124	92. 630	63. 449	31.455	1.00 16.84	В	С
ATOM	6714		TRP	124	91. 909	62. 942	33. 713	1.00 17.02	B	č
ATOM	6715		TRP	124	94. 819	62.999	31.539	1.00 19.00	В	č
ATOM	6716		TRP	124	93. 794	63. 429	30. 731	1.00 18.26	B	Ň
ATOM	6717		TRP	124	91. 331	63. 815	31.067	1.00 15.16	B	Ĉ
ATOM	6718		TRP	124	90.615	63.305	33. 326	1.00 16.85	B	Č
ATOM	6719	CH2	TRP	124	90. 342	63.737	32.011	1.00 16.12	B	Č
ATOM	6720	C	TRP	124	95.718	62.679	36. 427	1.00 17.28	B	Ċ
ATOM	6721	0	TRP	124	95.816	63.437	37.397	1.00 17.74	В	0
ATOM	6722	N	ARG	125	96.430	61.560	36.339	1.00 15.31	В	N
ATOM	6723	CA	ARG	125	97. 317	61.185	37.429	1.00 16.66	В	C
ATOM	6724	CB	ARG	125	97.666	59.702	37.323	1.00 16.96	В	С
ATOM	6725	CG	ARG	125	98. 908	59. 288	38.076	1.00 18.35	В -	C
ATOM	6726	CD	ARG	125	98.689	57.987	38.794	1.00 18.85	В	C
ATOM	6727	NE	ARG	125	98.049	56.965	37.972	1.00 18.57	В	N
ATOM	6728	CZ	ARG	125	97. 547	55.842	38.475	1.00 17.58	В	C
ATOM	6729	NH1		125	. 96.972	54.944	37.693	1.00 16.96	В	N
ATOM	6730		ARG	125	97.626	55.621	39. 776	1.00 17.03	B	N
ATOM	6731	C	ARG	125	98. 582	62.027	37.568	1.00 18.54	В	C
ATOM	6732	0	ARG	125	99.075	62.227	38.674	1.00 18.06	В	0
ATOM	6733	N	HIS	126	99. 099	62.533	36.454	$1.00\ 20.06$	В	N
ATOM	6734	CA	HIS	126	100.300	63. 353	36. 487	1.00 18.20	В	C
ATOM	6735	CB	HIS	126	101. 391	62.673	35. 673	1.00 18.72	В	C
ATOM	6736	CG	HIS	126	101.721	61. 295	36. 151	1.00 19.88	В	C
ATOM	6737		HIS	126	101.519	60.084	35. 581	1.00 20.06	В	C
ATOM	6738		HIS	126	102. 341	61.054	37. 360	1.00 17.75	В	· N
ATOM	6739		HIS	126	102.510	59. 753	37. 512	1.00 19.55	В	C
ATOM	6740		HIS	126	102.019	59. 142	36. 447	1.00 22.65	В	N
ATOM	6741	C	HIS	126	100.079	64. 772	35. 966	1.00 18.28	В	Č
ATOM	6742	0	HIS	126	100.692	65. 716	36. 462	1.00 18.27	В	0
ATOM	6743	N	SER	127	99. 204	64. 921	34. 974	1.00 16.08	В	N
ATOM	6744	CA	SER	127	98. 936	66. 230	34. 382	1.00 16.78	В	C
ATOM	6745 6746	CB	SER	127	98. 209	66.070	33. 037	1.00 15.96	В	C
ATOM ATOM	6747	OG C	SER SER	127		65. 349	33. 179		В	0
ATOM	6748	0	SER	127 127	98. 151 97. 523	67. 203	35. 261	1.00 16.75	В	C
ATOM	6749	N	TYR	128	98. 205	66. 816 68. 473	36. 247	1.00 17.88	В	0
ATOM	6750	CA	TYR	128	98. 203 97. 520	69. 556	34. 873	1.00 15.65	В	N
ATOM	6751	CB	TYR	128	97. 815	69. 506	35. 559 37. 060	1.00 17.91	В	C
ATOM	6752	CG	TYR	128	99. 253	69. 796	37. 444	1.00 17.70	В	C
ATOM	6753	CD1		128	99. 725	71. 107	37. 540	1.00 17.20 1.00 16.17	В	C
ATOM	6754		TYR	128	101.036	71. 375	37. 927	1.00 16.17	В	C
ATOM	6755		TYR	128	101. 030	68. 759	37. 739	1.00 10.04	B B	C C
ATOM	6756		TYR	128	100. 133	69.016	38. 123	1.00 17.12	В	C
ATOM	6757	CZ	TYR	128	101. 891	70. 322	38. 216	1.00 13.30	В	C
ATOM	6758	OH	TYR	128	103. 190	70. 572	38. 603	1.00 20.16	В	0
ATOM	6759	C	TYR	128	97. 977	70.897	34. 992	1.00 20.10	В	Č
ATOM	6760	Ŏ	TYR	128	98. 970	70. 972	34. 268	1.00 21.70	В	ŏ
ATOM	6761	N	THR	129	97. 239	71.955	35. 291	1.00 20.48	B	N

		FIG. 4-139	(Continued)
ATOM 67	72 O ALA 130 73 N SER 131 74 CA SER 131 75 CB SER 131 76 OG SER 131 77 C SER 131 78 O SER 131 79 N TYR 132 80 CA TYR 132 81 CB TYR 132 82 CG TYR 132 83 CD1 TYR 132 84 CE1 TYR 132 85 CD2 TYR 132 86 CE2 TYR 132 87 CZ TYR 132 88 OH TYR 132 89 C TYR 132 80 CA TYR 132 81 CB TYR 132 82 CG TYR 132 83 CD1 TYR 132 84 CE1 TYR 132 85 CD2 TYR 132 86 CE2 TYR 132 87 CZ TYR 132 88 OH TYR 132 89 C TYR 132 80 O TYR 132 80 O TYR 133 80 CA ASP 133 81 CB ASP 133 82 CA ASP 133 83 CB ASP 133	97. 647 73. 276 34. 840 1. 00 22. 26 96. 599 73. 968 33. 950 1. 00 23. 04 95. 353 74. 045 34. 652 1. 00 24. 93 96. 428 73. 213 32. 634 1. 00 22. 70 97. 856 74. 136 36. 069 1. 00 22. 23 97. 462 73. 765 37. 182 1. 00 20. 98 98. 474 75. 289 35. 854 1. 00 22. 77 98. 754 76. 222 36. 926 1. 00 23. 41 99. 789 75. 631 37. 859 1. 00 19. 73 99. 269 77. 525 36. 338 1. 00 26. 66 99. 514 77. 632 35. 133 1. 00 27. 20 99. 414 78. 523 37. 199 1. 00 29. 67 99. 934 79. 818 36. 796 1. 00 30. 14 99. 056 80. 948 37. 333 1. 00 30. 56 97. 713 80. 775 36. 913 1. 00 32. 67 101. 290 79. 851 37. 463 1. 00 31. 00 101. 448 79. 334 38. 569 1. 00 30. 79 102. 272 80. 438 36. 792 1. 00 32. 02 103. 611 80. 506 37. 347 1. 00 31. 40 104. 558 79. 634 36. 519 1. 00 28. 72 104. 179 78. 174 36. 516 1. 00 26. 74 103. 082 77. 721 35. 791 1. 00 26. 31 102. 696 76. 383 35. 834 1. 00 26. 58 104. 887 77. 250 37. 283 1. 00 26. 58 104. 887 77. 250 37. 283 1. 00 26. 58 104. 887 77. 250 37. 283 1. 00 26. 58 104. 887 77. 250 37. 283 1. 00 26. 58 104. 887 77. 250 37. 283 1. 00 26. 58 104. 887 77. 250 37. 283 1. 00 26. 58 104. 143 81. 929 37. 411 1. 00 32. 91 103. 743 82. 790 36. 636 1. 00 34. 01 105. 041 82. 165 38. 358 1. 00 35. 11 105. 674 83. 465 38. 539 1. 00 36. 35 104. 954 84. 287 39. 614 1. 00 38. 51 105. 674 83. 465 38. 539 1. 00 36. 35 104. 954 84. 287 39. 614 1. 00 38. 51 103. 732 85. 008 39. 074 1. 00 41. 22	Continued) B C B C B C B C B C B C B C B C B C B
ATOM 679 ATOM 679 ATOM 679	6 OD2 ASP 133	102. 805 84. 332 38. 580 1. 00 42. 20 103. 702 86. 253 39. 139 1. 00 42. 84	B 0 B 0
ATOM 679 ATOM 679 ATOM 680	8 0 ASP 133 9 N ILE 134 0 CA ILE 134	107. 112 83. 228 38. 954 1. 00 35. 61 107. 385 82. 438 39. 855 1. 00 35. 76 108. 031 83. 908 38. 285 1. 00 35. 21 109. 444 83. 764 38. 585 1. 00 34. 01	B C B O B N B C
ATOM 680; ATOM 680; ATOM 680; ATOM 680;	2 CG2 ILE 134 3 CG1 ILE 134 4 CD1 ILE 134 5 C ILE 134	110. 267 83. 750 37. 287 1. 00 33. 62 111. 718 83. 392 37. 593 1. 00 31. 90 109. 649 82. 737 36. 312 1. 00 32. 72 110. 204 82. 794 34. 909 1. 00 31. 29 109. 887 84. 911 39. 483 1. 00 34. 02	B C B C B C B C
ATOM 6800 ATOM 6800 ATOM 6800 ATOM 6810	7 N TYR 135 3 CA TYR 135 6 CB TYR 135	109. 521 86. 065 39. 261 1. 00 33. 25 110. 662 84. 573 40. 507 1. 00 35. 09 111. 167 85. 539 41. 475 1. 00 36. 09 110. 657 85. 174 42. 868 1. 00 36. 02 111. 222 86. 011 44. 000 1. 00 36. 66	B 0 B N B C B C B C

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					F I (S. 4 -	140			(Continued)
					1 1	J. I	1 10			
ATOM	6811	CD1		135	110.635	87. 222	44. 363	1.00 34.73	В	C
ATOM	6812		TYR	135	111. 134	87. 971	45. 424	1.00 34.55	В	C
ATOM	6813		TYR	135	112. 332	85. 573	44. 729	1.00 35.12	В	C
ATOM	6814		TYR	135	112. 839	86. 316	45. 786	1.00 35.07	В	C
ATOM	6815	CZ	TYR	135	112. 235	87. 515	46. 131	1.00 35.31	В	C
ATOM	6816	OH	TYR	135	112.740	88. 258	47. 179	1.00 35.05	В	0
ATOM	6817	C	TYR	135	112.688	85. 511	41.470	1.00 38.19	В	C
ATOM ATOM	6818 6819	O N	TYR ASP	135 136	113. 293	84. 517	41.873	1.00 37.81	B	0 N
ATOM	6820	CA	ASP	136	113. 304 114. 759	86. 600 86. 692	41.014 40.965	1.00 40.56 1.00 42.09	B B	N C
ATOM	6821	CB	ASP	136	115. 187	87. 969	40. 237	1.00 42.09	В	C C C
ATOM	6822	CG	ASP	136	116. 690	88. 051	40. 237	1.00 42.45	В	Ċ
ATOM	6823		ASP	136	117. 107	88. 577	38. 978	1.00 45.53	В	0
ATOM	6824		ASP	136	117. 456	87. 602	40.911	1.00 41.77	В	0
ATOM	6825	C	ASP	136	115. 316	86.679	42. 382	1.00 43.14	В	Č
ATOM	6826	Ŏ	ASP	136	114. 972	87. 522	43. 209	1.00 42.49	B	ŏ
ATOM	6827	Ň	LEU	137	116. 181	85. 713	42.656	1.00 44.92	B	Ň
ATOM	6828	CA	LEU	137	116.761	85.577	43.978	1.00 48.26	B	
ATOM	6829	CB	LEU	137	117. 219	84. 135	44. 182	1.00 48.88	В	C C C C
ATOM	6830	CG	LEU	137	116.058	83.136	44.117	1.00 49.07	В	Č
ATOM	6831		LEU	137	116.582	81.716	43.991	1.00 50.17	В	Č
ATOM	6832		LEU	137	115. 199	83. 291	45. 361	1.00 48.91	В	C
ATOM	6833	C	LEU	137	117. 908	86.544	44. 228	1.00 50.19	В	C
ATOM	6834	0	LEU	137	118. 309	86. 750	45.370	1.00 51.45	В	0
ATOM	6835	N	ASN	138	118. 429	87. 139	43.160	1.00 52.26	В	N
ATOM	6836	CA	ASN	138	119.522	88. 096	43. 280	1.00 53.21	В	C
ATOM	6837	CB	ASN	138	120. 330	88. 151	41.983	1.00 54.36	В	C
ATOM	6838	CG	ASN	138	120. 728	86.775	41.484	1.00 56.39	В	C
ATOM	6839		ASN	138	121. 232	85.945	42. 244	1.00 57.23	В	0
ATOM ATOM	6840 6841		ASN	138	120. 512	86.530	40. 194	1.00 56.67	В	N
ATOM	6842	C 0	ASN ASN	138 138	118. 935	89.472	43.567	1.00 54.11	В	C
ATOM	6843	N	LYS	139	119. 259 118. 064	90. 101 89. 929	44. 571 42. 675	1.00 54.39	В	0
ATOM	6844		LYS	139	117. 417			1.00 55.06 1.00 56.16	В	N C
ATOM	6845		LYS	139	116. 807	91.657	41.480	1.00 56.75	B B	C C
ATOM	6846	CG	LYS	139	117. 726	91.520	40. 290	1.00 58.34	В	C
ATOM	6847	CD	LYS	139	116. 996	91.874	39.006	1.00 59.63	В	Č
ATOM	6848	CE	LYS	139	117. 887	91.650	37. 793	1.00 61.32	В	č
ATOM	6849	NZ	LYS	139	117. 196	91.995	36. 518	1.00 62.59	В	Ň
ATOM	6850	C	LYS	139	116.302	91.183	43.857	1.00 56.78	B	Č
ATOM	6851	0	LYS	139	115.669	92. 202	44. 139	1.00 57.22	B	ŏ
ATOM	6852	N	ARG	140	116.061	90.006	44.425	1.00 57.14	B	N
ATOM	6853	CA	ARG	140	114. 994	89.838	45.409	1.00 57.44	В	Č
ATOM	6854	CB	ARG	140	115. 433	90.341	46.787	1.00 58.40	В	Č
ATOM	6855	CG	ARG	140	116.063	89. 260	47.649	1.00 61.65	В	C
ATOM	6856	CD	ARG	140	116.091	89.658	49.116	1.00 64.17	В	C
ATOM	6857	NE	ARG	140	116. 578	88. 575	49.972	1.00 67.20	В	N
ATOM	6858	CZ	ARG	140	115. 979	87. 394	50.112	1.00 68.02	В	C
ATOM	6859	NH1	ARG	140	114. 857	87.124	49. 453	1.00 68.21	В	N

		FIG. 4-141	(Continued)
1 5 10.		110. 4-141	
ATON ATON		140 116.507 86.478 50.911 1.00 68.11 B	N
ATON		140 113.697 90.537 44.994 1.00.56.16 B	Č
ATOM		140 113.067 91.225 45.795 1.00 56.03 B	0
ATOM		141 119 000 00 045 10 000 1.00 04,00 D	N
ATOM		1/1 119 907 09 900 10 TOO 1.00 00.90 D	C
ATOM	6866 CG GLN	141 119 100 00 000 11.00 00.10 B	C
ATOM		141 113.166 92.203 41.227 1.00 57.86 B 141 113.078 93.477 40.400 1.00 59.30 B	C C
ATOM		141 113.414 94.562 40.875 1.00 60.96 B	0
ATOM		141 112.620 93.350 39.158 1.00 58.33 B	N
ATOM ATOM		141 111.500 89.965 42.198 1.00 52.05 B	Ċ,
ATOM		141 112. 230 89. 362 41. 418 1. 00 52. 50 B	o '
ATOM		142 110.186 89.794 42.213 1.00 50.43 B 142 109.564 88.861 41.284 1.00 48.86 B	N
ATOM	6874 CB LEU	149 100 100 00 415 11.00 40.00 B	C
ATOM		149 107 094 00 005 41 075	C
ATOM	6876 CD1 LEU	142 107.024 89.395 41.857 1.00 48.67 B 142 106.354 89.442 40.489 1.00 49.83 B	C
ATOM		142 106.014 88.940 42.905 1.00 47.77 B	C C
ATOM ATOM		142 109.423 89.467 39.896 1.00 47.71 B	Č
ATOM		142 108. 890 90. 564 39. 736 1. 00 48. 46 B	ŏ
ATOM	0004	143 109. 917 88. 752 38. 891 1. 00 45. 67 B	N
ATOM		1/3 110 //9 90 900 90 707 1.00 42.90 B	C
ATOM	6883 CG2 ILE	1/3 110 204 00 CEO OF 202	C
ATOM	6884 CG1 ILE	143 111.937 88.055 36.810 1.00 41.53 B	C .
ATOM		143 112.675 87.257 35.755 1.00 42.12 B	C
ATOM ATOM		143 108. 385 89. 481 37. 131 1. 00 42. 92 B	Č
ATOM	2000	145 107. 522 88. 617 37. 292 1. 00 41. 84 B	Ŏ
ATOM	4444	106 700 01 005 00 000 1.00 40.07 B	N
ATOM	0000	44 106 222 02 244 20 015 1 00 44.00 B	C
ATOM	6891 OG1 THR 1	44 107 220 02 250 02 500 1.00 42.77 B	C
ATOM	6892 CG2 THR 1	44 106.124 92.080 38.388 1 00 43.33	0 C
ATOM ATOM		44 106.716 91.294 34.701 1.00 44.53 B	C
ATOM		44 105.689 91.729 34.186 1.00 46.08 B	Õ
ATOM	2000	45 107.802 90.988 34.001 1.00 45.05 B	N
ATOM		45. 100 060 09 091 00 000 1.00 40.00 B	C
ATOM	4000	45 100 140 02 210 20 207 1.00 JU. 14 B	C
ATOM	6899 CD GLU 1	45 110 420 04 004 00 000 1.00 JJ. 00 B	C
ATOM		45 110.696 94.443 31.591 1.00 60 26 R	C 0
ATOM ATOM	6901 OE2 GLU 14	45 . 111.167 94.357 33.737 1.00 59.47 B	0
ATOM	6902 C GLU 14 6903 O GLU 14	15 107. 946 89. 822 . 31. 834 1. 00 46. 87 B	C
ATOM	0004 17 -	108. 648 88. 916 32. 286 1. 00 46. 76 B	Ö
ATOM	6904 N GLU 14 6905 CA GLU 14	6 107 941 00 450 00 114 1.00 40.07 B	N
ATOM	6906 CB GLU 14	6 100 E00 00 004 00 000 1.00 40.04 B	C
ATOM	6907 CG GLU 14	6 100 010 00 001 20 100 TU TU TU	C
ATOM	6908 CD GLU 14	6 100 011 00 017 00 100 1.00 40.00 B	C C
			U

			FIG. 4-142	(Continued)
6931 6932 6933 6934 6935 6936 6937 6938 6939 6940 6941 6942 6943	OE1 GLU OE2 GLU O GLU N ARG CA ARG CB ARG CC ARG NE ARG CZ ARG NH1 ARG NH2 ARG C ARG ILE C ARG ILE CG1	146 146 146 147 147 147 147 147 147 147 147 148 148 148 148 149 149 149 149 149 150 150 150 150 150	107. 685 88. 081 26. 543 1. 00 45. 03 B 107. 641 90. 269 26. 387 1. 00 45. 44 B 106. 978 87. 241 30. 821 1. 00 46. 25 B 107. 805 86. 334 30. 912 1. 00 47. 62 B 105. 823 87. 221 31. 474 1. 00 44. 79 B 105. 475 86. 119 32. 360 1. 00 43. 34 B 104. 469 86. 595 33. 410 1. 00 44. 21 B 104. 998 87. 678 34. 320 1. 00 46. 85 B 103. 995 88. 007 35. 410 1. 00 49. 84 B 102. 805 88. 651 34. 866 1. 00 53. 22 B 101. 733 88. 970 35. 584 1. 00 53. 22 B 101. 696 88. 699 36. 884 1. 00 53. 97 B 104. 905 84. 894 31. 648 1. 00 54. 56 B 104. 304 84. 996 30. 580 1. 00 41. 06 B 105. 10	0 0 C 0 N C C C C N C N N C O N C C C C C C O N C C C C
6945 6946 6947 I	C ASN O ASN N ASN	150 150 151	97. 673 79. 929 32. 013 1. 00 30. 52 B 97. 722 79. 864 30. 777 1. 00 29. 37 B	C O N
5948 (5949 (5950 (5951 (5952 f 5953 (5954 (5955 f 5956 (CA ASN CB ASN CG ASN OD1 ASN ND2 ASN C ASN O ASN N THR CA THR	151 151 151 151 151 151 151 152 152	96. 859 77. 657 32. 170 1. 00 29. 53 B 95. 715 77. 881 31. 186 1. 00 33. 04 B 94. 489 78. 474 31. 850 1. 00 36. 73 B 94. 530 79. 586 32. 376 1. 00 38. 47 B 93. 389 77. 729 31. 831 1. 00 40. 28 B 98. 023 76. 997 31. 452 1. 00 28. 44 B 97. 856 76. 412 30. 382 1. 00 27. 56 B 99. 212 77. 111 32. 035 1. 00 26. 08 B 100. 384 76. 489 31. 452 1. 00 24. 37 B	N C C O N C O N C
	6910 6911 6911 6911 6911 6915 6916 6916 6917 6919 6920 6921 6922 6923 6924 6925 6926 6927 6928 6930 6931 6931 6931 6931 6931 6931 6931 6931	6909 OE1 GLU 6910 OE2 GLU 6911 C GLU 6912 O GLU 6913 N ARG 6914 CA ARG 6915 CB ARG 6916 CG ARG 6917 CD ARG 6918 NE ARG 6919 CZ ARG 6920 NH1 ARG 6921 NH2 ARG 6921 NH2 ARG 6921 C ARG 6922 C ARG 6923 O ARG 6924 N ILE 6925 CA ILE 6926 CB ILE 6927 CG2 ILE 6928 CG1 ILE 6929 CD1 ILE 6930 C ILE 6931 O ILE 6931 O ILE 6932 N PRO 6934 CA PRO 6935 CB PRO 6936 CG PRO 6937 C PRO 6936 CG PRO 6937 C PRO 6936 CA ASN 6940 CA ASN 6941 CB ASN 6941 CB ASN 6940 CA ASN 6941 CB ASN 6941 CB ASN 6941 CB ASN 6940 CA ASN 6941 CB ASN 6941 CB ASN 6941 CB ASN 6940 CA ASN 6941 CB ASN 6941 CB ASN 6940 CA ASN 6941 CB ASN 6940 CB ASN 6950 CG ASN 6951 OD1 ASN 6952 ND2 ASN 6955 N THR 6956 CA THR	6909 OE1 GLU 146 6910 OE2 GLU 146 6911 C GLU 146 6912 O GLU 146 6913 N ARG 147 6914 CA ARG 147 6915 CB ARG 147 6916 CG ARG 147 6917 CD ARG 147 6919 CZ ARG 147 6920 NH1 ARG 147 6920 NH1 ARG 147 6921 NH2 ARG 147 6922 C ARG 147 6923 O ARG 147 6924 N ILE 148 6925 CA ILE 148 6926 CB ILE 148 6927 CG2 ILE 148 6929 CD1 ILE 148 6929 CD1 ILE 148 6930 C ILE 148 6930 C ILE 148 6931 O ILE 148 6932 N PRO 149 6933 CD PRO 149 6933 CD PRO 149 6934 CA PRO 149 6935 CB PRO 149 6936 CG PRO 149 6937 C PRO 149 6937 C PRO 149 6938 O PRO 149 6938 O PRO 149 6939 N ASN 150 6940 CA ASN 150 6940 CA ASN 150 6941 CB ASN 150 6942 CG ASN 150 6944 ND2 ASN 150 6945 C ASN 150 6947 N ASN 151 6954 O ASN 151 6954 CB ASN 151 6954 CB ASN 151 6954 CB ASN 151 6955 N THR 152 6956 CA THR 152	6919 OEI GLU 146 107.685 88.081 26.543 1.00 45.03 B 6910 OB2 GLU 146 107.641 90.269 26.387 1.00 45.44 B 6911 C GLU 146 106.978 87.241 30.821 1.00 46.25 B 6912 O GLU 146 107.805 86.334 30.912 1.00 47.62 B 6913 N ARG 147 105.823 87.221 31.474 1.00 44.79 B 6914 CA ARG 147 105.475 86.119 32.360 1.00 43.34 B 6915 CB ARG 147 104.469 86.595 33.410 1.00 44.21 B 6916 CG ARG 147 104.998 87.678 34.320 1.00 46.85 B 6917 CD ARG 147 102.805 88.661 34.866 1.00 49.84 B 6918 NE ARG 147 102.805 88.661 34.866 1.00 49.84 B 6919 CZ ARG 147 101.733 88.970 35.584 1.00 54.21 B 6920 NH1 ARG 147 101.696 88.699 36.884 1.00 54.21 B 6921 NH2 ARG 147 100.701 89.569 34.999 1.00 54.56 B 6922 C ARG 147 104.908 87.32 32.259 1.00 38.31 B 6925 CA ILE 148 105.103 83.732 32.259 1.00 38.31 B 6925 CA ILE 148 105.103 83.732 32.259 1.00 38.31 B 6926 CB ILE 148 105.99 82.485 31.721 1.00 35.74 B 6920 CG ILE 148 106.599 82.485 31.721 1.00 35.74 B 6920 CG ILE 148 106.498 81.255 32.679 1.00 33.62 B 6920 CG ILE 148 106.599 82.485 31.721 1.00 35.74 B 6930 C ILE 148 100.495 83.155 32.664 1.00 35.07 B 6931 O ILE 148 100.495 83.155 32.664 1.00 35.61 B 6932 N PRO 149 100.942 82.321 30.526 1.00 31.27 B 6933 CD PRO 149 100.942 82.321 30.526 1.00 31.04 B 6934 CA SRO 149 100.942 82.321 30.526 1.00 31.27 B 6935 CB PRO 149 100.942 82.321 30.526 1.00 31.27 B 6936 CG PRO 149 100.942 82.321 30.526 1.00 31.27 B 6937 C PRO 149 100.942 82.321 30.526 1.00 31.27 B 6938 O PRO 149 100.942 82.321 30.526 1.00 31.99 B 6939 C CA SN 150 99.683 82.093 31.100 32.42 B 6930 C RASN 150 98.085 81.206 32.744 1.00 31.58 B 6931 O RASN 150 96.624 84.271 34.004 1.00 33.51 B 6934 CA SN 150 99.683 82.093 31.100 32.97 B 6939 C A SN 150 99.683 82.093 31.100 32.97 B 6934 CA SN 150 99.683 82.093 31.100 31.40 B 6935 CB SN 150 99.683 82.093 31.100 32.97 B 6936 CG PRO 149 100.87 81.549 31.592 1.00 31.48 B 6937 C ASN 150 99.683 82.073 31.00 31.95 B 6938 O PRO 149 100.87 81.549 31.592 1.00 31.48 B 6939 O CA SN 150 99.685 77.667 32.170 1.00 32.57 B 6940 CA SN 150 99.685 77.667 32.170 1.00 32.57 B 6940 CA S

			FIG. 4-143	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	6958 OG1 TH 6959 CG2 TH 6960 C TH 6961 O TH 6962 N GLI 6963 CA GLI 6964 CB GLI 6965 CG GLI 6966 CD GLI 6967 OE1 GLI 6968 NE2 GLI 6969 C GLI 6970 O GLI 6971 N TRI 6972 CA TRI 6972 CA TRI 6973 CB TRI 6974 CG TRI 6975 CD2 TRI 6975 CD2 TRI 6976 CE2 TRI 6976 CE2 TRI 6977 CE3 TRI 6977 CE3 TRI 6978 CD1 TRI 6979 NE1 TRI 6979 NE1 TRI 6980 CZ2 TRI 6981 CZ3 TRI 6981 CZ3 TRI 6982 CH2 TRI 6983 C TRI 6984 O TRI 6985 N VAL 6986 CA VAL 6987 CB VAL 6987 CB VAL 6987 CB VAL 6989 CG2 VAL 6989 CG2 VAL 6990 C VAL 6990 C VAL	R 152 R 152 153 153 153 153 153 153 153 154 154 154 154 154 154 154 154 154	101. 862 78. 407 31. 566 1. 00 25. 07 B 102. 882 76. 231 31. 643 1. 00 24. 98 B 100. 257 75. 012 31. 791 1. 00 22. 65 B 99. 908 74. 652 32. 912 1. 00 21. 72 B 100. 531 74. 160 30. 815 1. 00 21. 08 B 100. 407 72. 730 31. 010 1. 00 20. 14 B 100. 023 72. 081 29. 691 1. 00 20. 22 B 98. 688 72. 573 29. 166 1. 00 20. 23 B 99. 365 73. 054 26. 939 1. 00 21. 29 B 99. 365 73. 054 26. 939 1. 00 24. 47 B 97. 600 71. 703 27. 200 1. 00 20. 51 B 101. 650 72. 076 31. 578 1. 00 20. 86 B 101. 574 70. 996 32. 154 1. 00 22. 44 B 102. 794 72. 729 31. 422 1. 00 20. 43 B 104. 043 72. 189 31. 934 1. 00 18. 53 B 105. 678 </td <td></td>	
ATOM ATOM	6989 CG2 VAL 6990 C VAL	155 155	108. 180 76. 281 33. 260 1. 00 20. 89 B 108. 439 73. 255 33. 236 1. 00 21. 60 B	C C C
ATOM ATOM	6992 N THR 6993 CA THR	156 156	108. 241 72. 379 34. 075 1. 00 21. 26 B 109. 647 73. 590 32. 806 1. 00 22. 32 B 110. 826 72. 929 33. 325 1. 00 23. 44 B	O N C
ATOM ATOM ATOM	6994 CB THR 6995 OG1 THR 6996 CG2 THR	156 156 156	111.028 71.569 32.677 1.00 24.53 B 112.350 71.113 32.972 1.00 25.64 B 110.856 71.662 31.166 1.00 25.95 B	C 0 C
ATOM ATOM ATOM	6997 C THR 6998 O THR 6999 N TRP	156 156 157	112. 092 73. 727 33. 094 1. 00 24. 37 B 112. 305 74. 274 32. 010 1. 00 25. 56 B 112. 929 73. 795 34. 123 1. 00 23. 78 B	C 0
ATOM ATOM ATOM	7000 CA TRP 7001 CB TRP 7002 CG TRP	157 157 157	114.192 74.500 34.021 1.00 22.95 B 114.848 74.650 35.399 1.00 22.02 B	N C C
ATOM ATOM ATOM	7003 CD2 TRP 7004 CE2 TRP 7005 CE3 TRP	157 157	114.197 77.091 36.070 1.00 22.25 B 113.533 77.668 37.177 1.00 23.29 B	C C C
ATOM	7006 CD1 TRP	157 157	114. 658 77. 928 35. 046 1. 00 21. 12 B 113. 621 75. 460 37. 492 1. 00 22. 04 B	C C

				(Continued)
			FIG. 4-144	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	7007 NE1 TRI 7008 CZ2 TRI 7009 CZ3 TRI 7010 CH2 TRI 7011 C TRI 7012 O TRI 7013 N SEI 7014 CA SEI 7015 CB SEI 7016 OG SEI 7017 C SEI 7018 O SEI 7019 N PRO 7020 CD PRO 7021 CA PRO 7021 CA PRO 7022 CB PRO 7021 CA PRO 7022 CB PRO 7023 CG PRO 7024 C PRO 7025 O PRO 7026 N VAL 7027 CA VAL 7028 CB VAL 7027 CA VAL 7028 CB VAL 7029 CG1 VAL 7030 CG2 VAL 7031 C VAL 7030 CG2 VAL 7031 C VAL 7032 O VAL 7033 N GLY 7034 CA GLY 7035 C GLY 7036 O GLY 7037 N HIS 7038 CA HIS 7039 CB HIS 7040 CG HIS 7041 CD2 HIS 7041 CD2 HIS 7041 CD2 HIS	157 157 157 157 158 158 158 158 158 158 159 159 159 159 159 160 160	FIG. 4 - 144 113.193 76.650 38.030 1.00 22.01 B13.317 79.051 37.286 1.00 22.77 B114.445 79.299 35.156 1.00 22.58 B113.779 79.846 36.270 1.00 21.74 B15.096 73.640 33.153 1.00 22.79 B14.789 72.483 32.882 1.00 23.16 B16.198 74.211 32.697 1.00 21.93 B17.154 73.441 31.928 1.00 22.68 B18.104 74.377 31.172 1.00 23.20 B18.550 75.444 31.996 1.00 22.94 B17.898 72.667 33.017 1.00 23.12 B17.898 72.667 33.017 1.00 23.12 B17.898 72.667 33.017 1.00 23.12 B18.641 71.619 32.650 1.00 23.10 B18.927 71.096 31.307 1.00 23.10 B18.927 71.096 31.307 1.00 23.69 B19.362 70.860 33.679 1.00 24.10 B120.041 69.744 32.886 1.00 24.45 B119.230 69.660 31.599 1.00 23.97 B120.384 71.738 34.391 1.00 25.41 B120.598 71.619 35.589 1.00 26.39 B121.014 72.619 33.627 1.00 27.71 B122.031 73.517 34.146 1.00 29.28 B123.383 73.272 33.438 1.00 30.65 B124.421 74.249 33.939 1.00 33.70 B123.844 71.840 33.670 1.00 27.71 B122.031 73.517 34.146 1.00 29.28 B123.383 73.272 33.438 1.00 30.65 B124.421 74.249 33.939 1.00 33.70 B123.844 71.840 33.670 1.00 31.96 B122.043 75.866 34.745 1.00 29.32 B121.00 74.952 33.885 1.00 29.74 B120.889 75.224 32.923 1.00 30.93 B122.043 75.866 34.745 1.00 29.32 B121.706 77.266 34.562 1.00 28.43 B120.289 77.645 34.944 1.00 28.19 B19.839 77.359 36.053 1.00 30.02 B119.584 78.296 34.025 1.00 26.53 B18.222 78.721 34.290 1.00 25.12 B18.214 79.959 35.177 1.00 26.70 B119.019 81.094 34.629 1.00 29.24 B118.664 82.148 33.857 1.00 30.20 B118.664 82.148 33.857 1.00 30.29 95 B	N C C C C C C C C C C C C C C C C C C C
ATOM ATOM ATOM	7043 CE1 HIS 7044 NE2 HIS 7045 C HIS	162 162 162	120. 824 82. 283 34. 207 1. 00 30. 75 B 119. 804 82. 871 33. 608 1. 00 30. 77 B	C N
ATOM ATOM ATOM	7046 0 HIS 7047 N LYS 7048 CA LYS	162 163 163	117. 384 79. 021 33. 059 1. 00 24. 68 B 116. 730 80. 061 33. 007 1. 00 24. 17 B 117. 406 78. 135 32. 067 1. 00 22. 79 B 116. 575 78. 340 30. 889 1. 00 23. 10 B	C O N C
ATOM ATOM ATOM ATOM	7049 CB LYS 7050 CG LYS 7051 CD LYS 7052 CE LYS	163 163 163 163	117.113 77.578 29.675 1.00 22.90 B 118.367 78.184 29.063 1.00 23.40 B 118.797 77.407 27.841 1.00 22.69 B 120.103 77.930 27.282 1.00 23.67 B	C C C C
ATOM ATOM ATOM	7053 NZ LYS 7054 C LYS 7055 O LYS	163 163 163	120. 616 77. 045 26. 195 1. 00 24. 56 B 115. 215 77. 779 31. 266 1. 00 24. 15 B 115. 079 77. 104 32. 282 1. 00 24. 69 B	N C O

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					FIG. 4-145	(Continued)
					110. 1 110	
ATOM	7056		LEU	164	114. 210 78. 062 30. 450 1. 00 24. 82	B N
ATOM	7057			164	112.870 77.572 30.704 1.00 24.27	ВС
ATOM	7058		LEU	164	111. 991 78. 672 31. 293 1. 00 25. 27	ВС
ATOM	7059	CG		164	112. 216 78. 969 32. 769 1. 00 25. 61	ВС
ATOM	7060		1 LEU	164	111. 420 80. 181 33. 178 1. 00 25. 08	ВС
ATOM	7061		2 LEU	164	111. 802 77. 756 33. 582 1. 00 28. 15	B C
ATOM	7062		LEU	164	112. 231 77. 068 29. 435 1. 00 25. 20	B C
ATOM	7063		LEU	164	112. 438 77. 616 28. 353 1. 00 26. 77	B 0
ATOM	7064		ALA	165	111. 461 76. 003 29. 581 1. 00 24. 98	B N
ATOM	7065	CA	ALA	165	110. 736 75. 408 28. 479 1. 00 23. 92	B C
ATOM	7066	CB	ALA	165	111. 408 74. 127 28. 021 1. 00 23. 20	B C
ATOM	7067	C	ALA	165	109. 394 75. 106 29. 114 1. 00 25. 13	B C
ATOM ATOM	7068	0	ALA	165	109. 326 74. 494 30. 188 1. 00 24. 88	B 0
ATOM	7069	N	TYR	166	108. 326 75. 565 28. 481 1. 00 24. 06	B N
ATOM	7070 7071	CA CB	TYR	166	107.016 75.317 29.027 1.00 24.24	B C
ATOM	7072	CG	TYR	166	106.556 76.522 29.866 1.00 27.58	B C
ATOM	7073		TYR TYR	166	106. 370 77. 826 29. 115 1. 00 30. 69	B C
ATOM	7074		TYR	166	105. 171 78. 115 28. 465 1. 00 31. 46	B C
ATOM	7075		TYR	166 166	104. 981 79. 329 27. 800 1. 00 32. 97	B C
ATOM	7076		TYR	166	107. 386 78. 787 29. 077 1. 00 33. 05 107. 210 80. 005 28. 412 1. 00 34. 06	B C
ATOM	7077	CZ	TYR	166		B C
	7078	OH	TYR	166	105. 999 80. 270 27. 779 1. 00 34. 75 105. 789 81. 485 27. 162 1. 00 34. 83	B C
ATOM	7079	C	TYR	166	106.039 75.003 27.917 1.00 23.86	B O B C
ATOM	7080	0	TYR	166	106. 276 75. 333 26. 754 1. 00 22. 73	B C B O
ATOM	7081	N	VAL	167	104. 955 74. 321 28. 266 1. 00 22. 73	B N
ATOM	7082	CA	VAL	167	103. 960 73. 994 27. 269 1. 00 22. 82	B C
	7083	CB	VAL	167	103. 687 72. 487 27. 215 1. 00 21. 03	B C
	7084		VAL	167	102. 528 72. 200 26. 274 1. 00 17. 71	B C
	7085		VAL	167	104. 933 71. 770 26. 725 1. 00 20. 37	B C
	7086	C	VAL	167	102. 683 74. 754 27. 564 1. 00 23. 41	B C
	7087	0	VAL	167	102. 196 74. 779 28. 692 1. 00 24. 72	B 0
	7088	N	TRP	168	102. 162 75. 394 26. 531 1. 00 23. 89	B N
	7089	CA	TRP	168	100. 948 76. 179 26. 647 1. 00 24. 11	B C
	7090 7091	CB	TRP	168	101. 314 77. 664 26. 655 1. 00 24. 80	B C
	7092	CG CD2	TRP	168	100.171 78.550 26.958 1.00 27.20	B C
	7093	CE2		168	99. 572 79. 499 26. 075 1. 00 26. 49	B C
	7094	CE3		168 168	98. 496 80. 091 26. 769 1. 00 27. 49	B C .
	7095	CD1		168	99. 839 79. 907 24. 763 1. 00 27. 63	B C
	7096	NE1		168	99. 461 78. 602 28. 122 1. 00 27. 14	B C
	7097	CZ2		168	98. 452 79. 526 28. 017 1. 00 27. 81 97. 682 81. 074 26. 194 1. 00 26. 74	B N
	7098	CZ3		168		ВС
	7099	CH2		168	99.029 80.886 24.189 1.00 29.25 97.962 81.456 24.910 1.00 28.86	B C
	7100		TRP	168	100.072 75.838 25.444 1.00 22.93	B C
			TRP	168	100.577 75.692 24.328 1.00 21.98	B C B 0
ATOM 7			ASN	169	98. 768 75. 705 25. 675 1. 00 21. 44	B N
	7103		ASN	169	97. 830 75. 350 24. 610 1. 00 22. 01	B C
ATOM 7	7104		ASN	169	97. 394 76. 580 23. 813 1. 00 23. 30	B C
					1.00 20.00	~ ·

ATOM 7105 CG ASN 169 96.682 77.615 24.662 1.00 27.95 B C ATOM 7107 ND2 ASN 169 96.240 78.640 24.150 1.00 32.66 B O ATOM 7107 ND2 ASN 169 98.463 74.345 23.655 1.00 21.23 B C ATOM 7109 ASN 169 98.463 74.345 23.655 1.00 21.23 B C ATOM 7109 ASN 169 98.463 74.541 22.441 1.00 22.01 B O ATOM 7110 N ASN 170 99.031 73.283 24.221 1.00 20.60 B N ATOM 71110 N ASN 170 99.61 72.208 23.459 1.00 20.97 B C ATOM 71110 CA ASN 170 99.61 72.208 23.459 1.00 20.97 B C ATOM 71112 CB ASN 170 99.61 72.208 23.459 1.00 20.97 B C ATOM 7112 CB ASN 170 97.629 70.741 23.412 1.00 18.68 B C ATOM 7113 CG ASN 170 97.629 70.741 23.412 1.00 18.15 B C ATOM 7114 0D1 ASN 170 97.158 71.224 24.440 1.00 16.27 B O ATOM 7115 ND2 ASN 170 97.000 65.529 22.966 1.00 21.31 B C ATOM 7116 ND2 ASN 170 97.000 65.529 22.966 1.00 18.92 B N ATOM 7116 ND2 ASN 170 97.000 65.529 22.966 1.00 21.31 B C ATOM 7118 N ASP 171 101.504 73.697 22.915 1.00 22.16 B N ATOM 7118 N ASP 171 101.504 73.697 22.916 1.00 23.35 B C ATOM 7118 N ASP 171 101.504 73.697 22.916 1.00 23.35 B C ATOM 7120 CB ASP 171 102.507 74.122 22.160 1.00 23.35 B C ATOM 7120 CB ASP 171 102.507 74.122 22.160 1.00 23.72 B C ATOM 7122 001 ASP 171 102.507 74.383 91.00 23.72 B C ATOM 7122 001 ASP 171 102.507 74.383 91.00 23.72 B C ATOM 7123 002 ASP 171 102.505 74.380 23.073 1.00 23.59 B C ATOM 7124 C ASP 171 102.505 74.380 23.73 1.00 23.59 B C ATOM 7125 O ASP 171 103.850 74.380 23.073 1.00 23.59 B C ATOM 7127 C ASP 171 103.850 74.380 23.073 1.00 23.59 B C ATOM 7128 CB ILE 172 105.651 74.301 22.508 1.00 23.60 B N ATOM 7127 C AILE 172 105.651 74.301 22.508 1.00 23.60 B N ATOM 7127 C AILE 172 106.672 74.497 23.281 1.00 23.66 B C ATOM 7133 O ILE 172 107.707 70.986 22.374 1.00 23.66 B C ATOM 7133 O ILE 172 107.707 70.986 22.374 1.00 23.66 B C ATOM 7133 C ILE 172 107.707 70.986 22.385 1.00 23.66 B C ATOM 7133 C ILE 172 107.707 70.986 22.374 1.00 23.66 B C ATOM 7144 C TYR 173 103.497 73.897 66.414 24.236 1.00 23.66 B C ATOM 7144 C TYR 173 103.492 73.897 66.414 24.236 1.00 23.65 B C ATOM 7144 C TYR 173 103.492 73.897 66.414		-				F I	G. 4	146			(Continued)
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ALOM 1.00 A D.LO [[] []A.444 [M.MM] A.[. []MM [. UI] XM [X K N	ATOM	7153	N	LYS	175	111. 767	79. 990	27. 099	1.00 31.81	В	U N

					FIG	. 4 -	147			(Continued)
ATOM	7154			175	112.940	81. 269	27. 608	1.00 28.47	В	С
ATOM	7155			175	112.090	81.725	28. 794		В	С
ATOM	7156			175	110.809	82.428	28. 413		В	C
ATOM ATOM	7157 7158			175	109.876	82.551	29. 611	1.00 32.27	В	Č
ATOM	7159		LYS LYS	175 175	110.479	83. 384	30. 725	1.00 31.57	В	C
ATOM	7160		LYS	175	110.664 114.382	84. 791	30. 307	1.00 33.57	В	N
ATOM	7161	0	LYS	175	114. 362	81.107 80.355	28. 064 28. 999	1.00 28.80 1.00 28.36	B B	C
ATOM	7162	Ň	ILE	176	115. 294	81.813	27. 401	1.00 28.58	В	O N
ATOM	7163	CA		176	116.710	81. 764	27. 749	1.00 28.19	В	C
ATOM	7164	CB		176		82. 363	26. 624	1.00 27.21	В	č
ATOM	7165	CG	2 ILE	176	118. 942	82.730	27. 146	1.00 25.54	B	č
ATOM	7166		ILE	176		81.354	25.483	1.00 28.29	В	С
ATOM	7167		1 ILE	176		80.941	24.861	1.00 27.38	В	C
ATOM ATOM	7168 7169	C 0	ILE	176		82. 528	29.044	1.00 29.36	В	C
ATOM	7170	N	ILE GLU	176 177		82. 251	29. 768	1.00 29.16	В	0
ATOM	7171	CA	GLU	177		83. 489 84. 296	29. 330	1.00 31.44	В	N
ATOM	7172	CB	GLU	177		85.611	30. 543 30. 241	1.00 33.96 1.00 35.87	B B	C
ATOM	7173	CG	GLU	177		85. 440	29. 770	1.00 35.67	B B	C C
ATOM	7174	CD	GLU	177		85. 272	30.916	1.00 39.82	В	C
ATOM	7175		GLU	177		84. 988	30.642	1.00 40.62	B	ŏ
ATOM	7176		GLU GLU	177	118.914	85. 433	32.088	1.00 40.43	B	Ö
ATOM	7177	C	GLU	177		84. 569	31.034	1.00 34.61	В	С
ATOM ATOM	7178	0	GLU	177		85. 007	30. 268	1.00 35.24	В	0
ATOM	7179 7180	N CD	PRO PRO	178 178	114.495	84. 312	32. 323	1.00 35.55	В	N
ATOM	7181	CA	PRO	178		83. 907 84. 530	33. 367	1.00 36.07	В	C
ATOM	7182	CB	PRO	178		84. 357	32. 894 34. 402	1.00 35.46 1.00 35.40	В	C
ATOM	7183	ĊĠ	PRO	178		84. 563	34. 587	1.00 35.40	B B	C C
ATOM	7184	C	PRO	178		85. 834	32. 547	1.00 31.12	В	C
ATOM	7185	0	PRO	178		85. 859	32. 446	1.00 35.44	В	Ö
ATOM	7186	N	ASN	179	113.198	36. 912	32.346	1.00 36.89	B	Ň
ATOM	7187	CA	ASN	179			32.021	1.00 37.31	В	Ċ
ATOM	7188	CB	ASN	179	113. 211 8	39. 329		1.00 37.54	В	C
ATOM ATOM	7189 7190	CG	ASN	179			32. 137	1.00 37.86	В	C
ATOM	7190		ASN ASN	179			31.915	1.00 39.14	В	0
ATOM	7192	C	ASN	179 179			31.806	1.00 40.48	В	N
ATOM	7193	Õ	ASN	179			30. 535 30. 159	1.00 36.88 1.00 38.11	В	C
ATOM	7194	Ň	LEU	180			29. 689	1.00 35.31	В В	O N
ATOM	7195	CA	LEU	180			28. 260	1.00 33.31	В	C
ATOM	7196	CB	LEU	180			27. 662	1.00 35.92	В	Č
ATOM	7197	CG	LEU	180			28. 279	1.00 36.91	B	č
ATOM	7198		LEU	180	116.828 8	7. 572	27.470	1.00 37.09	B	č .
ATOM	7199		LEU	180			28. 303	1.00 37.24	В	С
ATOM	7200	C	LEU	180			27. 547	1.00 33.52	В	С
ATOM	7201	0 N	LEU	180			28. 015	1.00 32.50	В	0
ATOM	7202	N	PRO	181	111.462 8	7. 704	26. 400	1.00 34.20	В	N

	<u>.</u>		FIG. 4-148	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	7203 CD PRO 7204 CA PRO 7205 CB PRO 7206 CG PRO 7207 C PRO 7208 O PRO 7209 N SEI 7210 CA SEI 7211 CB SEI 7212 OG SEI 7213 C SEI 7214 O SEI 7214 O SEI 7215 N TYR 7216 CA TYR 7217 CB TYR 7217 CB TYR 7218 CG TYR 7219 CD1 TYR 7220 CE1 TYR 7221 CD2 TYR 7222 CE2 TYR	181 181 181 181 181 181 182 182 182 182	108. 752 82. 622 25. 547 1. 00 31. 33 107. 505 82. 817 24. 909 1. 00 30. 50 109. 759 83. 117 23. 350 1. 00 31. 89 109. 077 83. 812 22. 606 1. 00 33. 14 110. 463 82. 077 22. 927 1. 00 31. 53 110. 453 81. 677 21. 532 1. 00 30. 47 111. 832 81. 159 21. 118 1. 00 30. 68 112. 962 82. 117 21. 408 1. 00 32. 75 113. 490 82. 235 22. 696 1. 00 32. 39 114. 517 83. 134 22. 977 1. 00 33. 30 113. 492 82. 926 20. 398 1. 00 33. 06 114. 520 83. 832 20. 667 1. 00 34. 20	B C B C B C B C B C B C B C B C B C B C
ATOM ATOM ATOM	7223 CZ TYR 7224 OH TYR 7225 C TYR	183	115. 028 83. 932 21. 959 1. 00 34. 92 116. 036 84. 832 22. 233 1. 00 34. 60	B 0
ATOM	7226 0 TYR	183 183		B C
ATOM	7227 N ARG	184	100 570 00 050 00 000	B O B N
ATOM	7228 CA ARG	184	107. 573 79. 631 20. 148 1. 00 26. 57	
ATOM	7229 CB ARG	184	106.327 80.217 19.476 1.00 26.06	
ATOM ATOM	7230 CG ARG 7231 CD ARG	184	105. 215 79. 191 19. 285 1. 00 28. 64 E	
ATOM	7231 CD ARG 7232 NE ARG	184 184	103. 860 79. 825 19. 004 1. 00 30. 29	3 C
ATOM	7233 CZ ARG	184	102. 827 78. 805 18. 831 1. 00 31. 47 101. 526 79. 052 18. 706 1. 00 29. 99	
ATOM	7234 NH1 ARG	184	100 000 000 000	
ATOM	7235 NH2 ARG	184	100. 678 78. 048 18. 552 1. 00 30. 76 B	
ATOM	7236 C ARG	184	108. 185 78. 553 19. 272 1. 00 26. 51 B	
ATOM ATOM	7237 0 ARG	184	108. 375 78. 754 18. 072 1. 00 28. 42 B	
ATOM	7238 N ILE 7239 CA ILE	185	108. 493 77. 411 19. 876 1. 00 24. 50 B	N
ATOM	7240 CB ILE	185 185	109. 112 76. 303 19. 165 1. 00 22. 88 B 109. 773 75. 319 20. 159 1. 00 23 12 B	
ATOM	7241 CG2 ILE	185	110 400 74 010 10 10	
ATOM	7242 CG1 ILE	185	110 700 70 000	
ATOM	7243 CD1 ILE	185	111. 869 76. 770 20. 324 1. 00 21. 93 B	
ATOM	7244 C ILE	185	108.148 75.516 18.275 1.00 24.00 B	
ATOM ATOM	7245 O ILE 7246 N THR	185	108. 569 74. 930 17. 275 1. 00 25. 07 B	Ŏ
ATOM	7246 N THR 7247 CA THR	186 186	106. 866 75. 489 18. 632 1. 00 22. 70 B 105. 886 74. 750 17. 840 1. 00 23 30 B	. N
ATOM	7248 CB THR	186	105 400 50 440	C
ATOM	7249 OG1 THR	186	100 000 00 000	C
ATOM	7250 CG2 THR	186	105. 058 73. 727 19. 877 1. 00 27. 42 B 106. 665 72. 491 18. 595 1. 00 19. 86 B	0 C
ATOM	7251 C THR	186	104. 620 75. 548 17. 537 1. 00 23. 45 B	C

		FIG. 4-149	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	1 7253 N TRP 1 7254 CA TRP 1 7255 CB TRP 7256 CG TRP 7257 CD2 TRP 7258 CE2 TRP 7259 CE3 TRP 7260 CD1 TRP 7261 NE1 TRP 7262 CZ2 TRP 7263 CZ3 TRP 7264 CH2 TRP 7265 C TRP 7266 O TRP 7267 N THR 7268 CA THR 7270 OG1 THR 7271 CG2 THR 7272 C THR 7273 O THR 7274 N GLY 7275 CA GLY 7276 C GLY 7279 CA LYS 7280 CB LYS 7281 CG LYS <	186 104. 266 76. 469 18. 265 1. 00 22. 05 187 103. 935 75. 179 16. 457 1. 00 24. 88 187 102. 717 75. 876 16. 049 1. 00 25. 32 187 103. 007 76. 767 14. 832 1. 00 25. 43 187 104. 159 77. 694 15. 025 1. 00 25. 95 187 104. 093 79. 092 15. 321 1. 00 26. 73 187 105. 420 79. 548 15. 464 1. 00 26. 07 187 105. 420 79. 548 15. 464 1. 00 26. 07 187 105. 420 79. 548 15. 464 1. 00 26. 93 187 105. 485 77. 367 15. 019 1. 00 26. 93 187 105. 485 77. 367 15. 019 1. 00 26. 93 187 106. 249 78. 474 15. 298 1. 00 26. 08 187 103. 346 81. 332 15. 764 1. 00 26. 71 187 104. 679 81. 751 15. 922 1. 00 25. 13 187 104. 679 81. 751 15. 922 1. 00 26. 58	B O N B B C C B B C C C B B B B B B B B B B
ATOM ATOM		91 92. 461 71. 475 22. 728 1. 00 26. 71 B	C
ATOM ATOM	7291 CD GLU 19	91 90. 752 71. 859 24. 514 1. 00 34. 15 B	C C
ATOM	7292 OE1 GLU 19 7293 OE2 GLU 19	00 FF1 70 000 1.00 00.40 B	0
ATOM	7294 C GLU 19		0
ATOM	7295 0 GLU 19	91 92.031 69.280 20.713 1.00 20.17 B	C 0
ATOM ATOM	7296 N ASP 19 7297 CA ASP 19	92 93. 208 68. 157 22. 287 1. 00 23. 70 B	N
ATOM	7297 CA ASP 19 7298 CB ASP 19	92. 707 66. 811 21. 996 1. 00 24. 98 B	C
ATOM	7299 CG ASP 19	19 00 700 CT 100 ZL. 140 1.00 ZL. Zt	C
ATOM	7300 OD1 ASP 19		C 0

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	FIG. 4-150											
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	7301 OD2 AS 7302 C AS 7303 O AS 7304 N IL 7305 CA IL 7306 CB IL 7307 CG2 IL 7308 CG1 IL 7310 C ILI 7311 O ILI 7312 N ILI 7313 CA ILI 7314 CB ILI 7315 CG2 ILI 7316 CG1 ILI 7317 CD1 ILI 7318 C ILI 7317 CD1 ILI 7318 C ILI 7319 O ILI 7319 O ILI 7319 CA TYP 7320 N TYP 7321 CA TYP 7320 N TYP 7321 CA TYP 7322 CB TYP 7323 CG TYP 7324 CD1 TYP 7325 CE1 TYP 7326 CD2 TYP 7327 CE2 TYP 7328 CZ TYP 7329 OH TYP 7320 N TYP 7321 CA TYP 7321 CA TYP 7322 CB TYP 7323 CG TYP 7324 CD1 TYP 7325 CE1 TYP 7326 CD2 TYP 7327 CE2 TYP 7328 CZ TYP 7328 CZ TYP 7329 OH TYP 7330 C TYP 7331 O TYP 7331 O TYP 7332 N ASN 7333 CA ASN 7334 CB ASN 7335 CG ASN	P 192 P 193 193 193 193 193 193 193 193 194 194 194 194 194 194 195 195 195 195 195 195	89. 671 67. 908 23. 548 1. 00 32. 44 93. 072 66. 329 20. 602 1. 00 25. 95 92. 431 65. 426 20. 065 1. 00 27. 81 94. 091 66. 926 20. 000 1. 00 25. 46 94. 485 66. 512 18. 665 1. 00 25. 50 93. 970 67. 502 17. 595 1. 00 26. 97 94. 426 67. 057 16. 212 1. 00 26. 11 92. 441 67. 552 17. 621 1. 00 27. 90 91. 784 66. 246 17. 210 1. 00 29. 23 95. 994 66. 390 18. 546 1. 00 25. 04 96. 519 65. 297 18. 334 1. 00 22. 43 98. 139 67. 505 18. 589 1. 00 21. 47 98. 618 68. 429 17. 456 1. 00 21. 58 100. 146 68. 414 17. 377 1. 00 18. 60 97. 972 68. 001 16. 133 1. 00 15. 81 98. 79 67. 968 19.	Continued) B O B C B C B C B C B C B C B C B C B C								
ATOM ATOM	7336 OD1 ASN 7337 ND2 ASN	196 196	103. 769 69. 311 18. 632 1. 00 17. 04 102. 362 70. 943 19. 267 1. 00 17. 01	B C B O B N								
ATOM ATOM ATOM	7338 C ASN 7339 O ASN 7340 N GLY	196 196 197	104. 380 69. 160 23. 104 1. 00 18. 89 103. 976 70. 066 23. 828 1. 00 21. 80 105. 355 68. 344 23. 479 1. 00 18. 21	B C B O B N								
ATOM ATOM ATOM	7341 CA GLY 7342 C GLY 7343 O GLY	197 197 197	105. 976 68. 533 24. 778 1. 00 18. 42 105. 185 67. 948 25. 941 1. 00 18. 43	B C C								
ATOM ATOM	7344 N ILE 7345 CA ILE	198 198	103. 976 67. 469 25. 654 1. 00 15. 16 103. 129 66. 842 26. 667 1. 00 14. 58	B O B N B C								
ATOM ATOM ATOM	7346 CB ILE 7347 CG2 ILE 7348 CG1 ILE	198 198 198	101. 956 67. 740 27. 160 1. 00 12. 66 102. 477 68. 784 28. 109 1. 00 10. 73	B C C								
ATOM	7349 CD1 ILE	198	00 000	B C								

					FIG. 4-151	(Continued)
					110. 4 101	
ATOM	7350		ILE	198	102. 523 65. 585 26. 101 1. 00 14. 46 B	C
ATOM ATOM	7351 7352		ILE THR	198 199	102. 354 65. 447 24. 895 1. 00 16. 78 B	0
ATOM	7353			199	102. 182 64. 671 26. 990 1. 00 15. 77 B 101. 600 63. 396 26. 608 1. 00 15. 94 B	N
ATOM	7354			199	101. 600 63. 396 26. 608 1. 00 15. 94 B 101. 982 62. 350 27. 630 1. 00 15. 69 B	C
ATOM	7355			199	101. 683 62. 861 28. 937 1. 00 12. 99 B	0
ATOM	7356		2 THR	199	103. 473 62. 043 27. 534 1. 00 15. 54 B	č
ATOM	7357		THR	199	100. 085 63. 448 26. 522 1. 00 15. 87 B	č
ATOM	7358		THR	199	99. 452 64. 311 27. 133 1. 00 16. 77 B	0
ATOM ATOM	7359		ASP	200	99. 510 62. 534 25. 745 1. 00 16. 29 B	N
ATOM	7360 7361	CA CB		$\begin{array}{c} 200 \\ 200 \end{array}$	98. 058 62. 450 25. 619 1. 00 16. 42 B	C
ATOM	7362	CG		200	97. 654 61. 812 24. 279 1. 00 17. 56 B 97. 960 60. 321 24. 207 1. 00 19. 40 B	C
ATOM	7363		1 ASP	200	97. 960 60. 321 24. 207 1. 00 19. 40 B 98. 894 59. 847 24. 892 1. 00 20. 07 B	C 0
ATOM	7364		2 ASP	200	97. 267 59. 624 23. 438 1. 00 19. 79 B	0
ATOM	7365	C	ASP	200	97. 657 61. 578 26. 806 1. 00 15. 56 B	Č
ATOM	7366	0	ASP	200	98. 502 61. 278 27. 648 1. 00 16. 67 B	ŏ
ATOM	7367	N	TRP	201	96. 404 61. 151 26. 889 1. 00 14. 09 B	N
ATOM ATOM	7368 7369	CA	TRP	201	96. 003 60. 368 28. 049 1. 00 13. 08 B	C
ATOM	7370	CB CG	TRP TRP	201 201	94. 503 60. 106 28. 037 1. 00 13. 25 B	C
ATOM	7371		TRP	201	94. 023 59. 554 29. 348 1. 00 12. 63 B 94. 135 58. 198 29. 801 1. 00 10. 35 B	C
ATOM	7372		TRP	201	94. 135 58. 198 29. 801 1. 00 10. 35 B 93. 610 58. 150 31. 110 1. 00 11. 08 B	C
ATOM	7373		3 TRP	201	94. 634 57. 020 29. 228 1. 00 8. 52 B	C C C C C C
ATOM	7374		TRP	201	93. 449 60. 253 30. 370 1. 00 12. 43 B	Č
ATOM	7375		TRP	201	93. 198 59. 416 31. 434 1. 00 12. 21 B	Ň
ATOM	7376		TRP	201	93. 567 56. 967 31. 858 1. 00 11. 85 B	
ATOM ATOM	7377 7378		TRP	201	94. 596 55. 847 29. 968 1. 00 8. 91 B	C C C
ATOM	7379	C	TRP	201 201	94. 065 55. 829 31. 271 1. 00 10. 19 B 96. 719 59. 040 28. 264 1. 00 14. 63 B	C
ATOM	7380	ŏ	TRP	201	07 107 70 700	
ATOM	7381	Ň	VAL	202	97. 197 58. 766 29. 366 1. 00 14. 84 B 96. 795 58. 213 27. 224 1. 00 14. 84 B	O N
ATOM	7382	CA	VAL	202	97. 413 56. 902 27. 369 1. 00 13. 74 B	
ATOM	7383	CB	VAL	202	97. 028 55. 966 26. 190 1. 00 11. 30 B	C C
ATOM	7384		VAL	202	97. 960 56. 155 25. 010 1. 00 8. 57 B	Č
ATOM ATOM	7385 7386		VAL	202	97. 028 54. 541 26. 667 1. 00 8. 82 B	С
ATOM	7387	C 0	VAL VAL	202 202	98. 929 56. 920 27. 556 1. 00 15. 45 B	Č
ATOM	7388	N	TYR	202	99. 471 56. 095 28. 292 1. 00 16. 05 B 99. 616 57. 857 26, 906 1. 00 15. 45 B	0
ATOM	7389	CA	TYR	203	99. 616 57. 857 26, 906 1. 00 15. 45 B 101. 060 57. 941 27. 053 1. 00 13. 39 B	N
ATOM	7390	CB	TYR	203	101.656 58.918 26.035 1.00 12.37 B	C C
ATOM	7391	CG	TYR	203	102. 248 58. 238 24. 823 1. 00 8. 90 B	Č
ATOM	7392		TYR	203.	101. 461 57. 938 23. 709 1. 00 8. 82 B	Č
ATOM	7393		TYR	203	101. 989 57. 260 22. 619 1. 00 7. 48 B	č
ATOM ATOM	7394 7395	CD2		203	103. 587 57. 844 24. 812 1. 00 5. 53 B	C
ATOM	7396	CE2 CZ	TYR	203 203	104.128 57.167 23.727 1.00 6.51 B	C
ATOM	7397	OH	TYR	203 203	103. 325 56. 874 22. 634 1. 00 8. 49 B 103. 849 56. 175 21. 572 1. 00 8. 01 B	C
ATOM	7398	C	TYR	203	101 100	0
		-		200	101. 438 58. 371 28. 471 1. 00 13. 68 B	С

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				FIG. 4-152	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	7399 7400 7401 7402 7403 7404 7405	N GLU CA GLU CB GLU	203 204 204 204 204 204 204	102. 369 57. 832 29. 056 1. 00 12. 65 B 100. 706 59. 335 29. 020 1. 00 15. 26 B 100. 963 59. 827 30. 376 1. 00 16. 69 B 99. 975 60. 936 30. 743 1. 00 16. 67 B 100. 174 61. 457 32. 161 1. 00 17. 47 B 98. 950 62. 154 32. 731 1. 00 17. 71 B 98. 197 62. 785 31. 964 1. 00 19. 00 B	0 N C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	7406 7407 7408 7409 7410 7411 7412 7413	OE2 GLU C GLU N GLU CA GLU CB GLU CG GLU CD GLU	204 204 204 205 205 205 205 205	98. 753 62. 085 33. 962 1. 00 18. 59 B 100. 831 58. 740 31. 437 1. 00 17. 37 B 101. 681 58. 597 32. 305 1. 00 18. 22 B 99. 745 57. 980 31. 353 1. 00 18. 89 B 99. 442 56. 932 32. 315 1. 00 19. 55 B 97. 925 56. 727 32. 344 1. 00 20. 80 B 97. 453 55. 436 32. 995 1. 00 23. 74 B 97. 414 55. 494 34. 515 1. 00 26. 68 B	0 C O N C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	7414 7415 7416 7417 7418 7419 7420 7421	OE1 GLU OE2 GLU C GLU O GLU N GLU CA GLU CB GLU CG GLU	205 205 205 205 205 206 206 206 206	97. 038 54. 466 35. 118 1. 00 28. 71 B 97. 744 56. 547 35. 106 1. 00 26. 12 B 100. 132 55. 578 32. 131 1. 00 19. 27 B 100. 525 54. 957 33. 107 1. 00 19. 31 B 100. 291 55. 124 30. 893 1. 00 18. 93 B 100. 876 53. 808 30. 660 1. 00 18. 63 B 99. 989 53. 016 29. 705 1. 00 18. 05 B	0 0 C 0 N C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	7422 7423 7424 7425 7426 7427 7428	CD GLU OE1 GLU OE2 GLU C GLU O GLU N VAL CA VAL	206 206 206 206 206 206 207 207	98. 535 52. 921 30. 139 1. 00 20. 39 B 98. 359 52. 143 31. 422 1. 00 20. 74 B 97. 205 51. 905 31. 821 1. 00 21. 45 B 99. 375 51. 768 32. 037 1. 00 22. 90 B 102. 293 53. 766 30. 136 1. 00 19. 32 B 102. 976 52. 761 30. 292 1. 00 20. 01 B 102. 744 54. 844 29. 509 1. 00 20. 90 B 104. 092 54. 855 28. 968 1. 00 20. 95 B	C C O C O N C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	7429 7430 7431 7432 7433 7434 7435 7436	CB VAL CG1 VAL CG2 VAL C VAL O VAL N PHE CA PHE CB PHE	207 207 207 207 207 208 208 208	104. 101 55: 347 27. 509 1. 00 21. 52 B 105. 486 55. 151 26. 918 1. 00 22. 17 B 103. 048 54. 592 26. 684 1. 00 19. 10 B 105. 080 55. 691 29. 775 1. 00 21. 67 B 106. 052 55. 160 30. 301 1. 00 25. 32 B 104. 833 56. 989 29. 888 1. 00 21. 55 B 105. 743 57. 870 30. 611 1. 00 21. 33 B	C C C O N C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	7437 7438 7439 7440 7441 7442 7443	CG PHE CD1 PHE CD2 PHE CE1 PHE CE2 PHE CZ PHE C PHE	208 208 208 208 208 208 208 208	105. 877 59. 201 29. 863 1. 00 21. 28 B 106. 571 59. 083 28. 536 1. 00 21. 92 B 107. 890 58. 649 28. 464 1. 00 20. 63 B 105. 893 59. 373 27. 353 1. 00 22. 58 B 108. 525 58. 499 27. 230 1. 00 22. 52 B 106. 521 59. 225 26. 109 1. 00 22. 24 B 107. 837 58. 787 26. 048 1. 00 22. 76 B 105. 444 58. 168 32. 082 1. 00 21. 89 B	C C C C C C
ATOM ATOM ATOM ATOM	7444 7445 7446 7447	O PHE N SER CA SER CB SER	208 209 209 209	106. 298 58. 727 32. 768 1. 00 23. 07 B 104. 261 57. 811 32. 577 1. 00 20. 48 B 103. 922 58. 094 33. 976 1. 00 19. 86 B 104. 689 57. 165 34. 905 1. 00 18. 09 B	O N C C

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					FIG	4 -	153			(Continued)
ATOM	7448	0G	SER	209		55.820	34.601	1.00 21.42	В	0
ATOM	7449	Ċ	SER			59. 543	34. 286	1.00 20.55	B	č
ATOM	7450	0	SER			59.877	35.367	1.00 19.53	В	0
ATOM	7451	N	ALA			60.394	33. 302	1.00 20.69	В	N
ATOM	7452	CA	ALA	210		61.809	33.393	1.00 20.47	В	C
ATOM	7453	CB	ALA			62.044	33. 228	1.00 20.63	В	C
ATOM	7454	C	ALA	210		62. 492	32. 275	1.00 20.53	В	C
ATOM	7455	0 N	ALA	210		61.835	31.367	1.00 19.81	В	0
ATOM ATOM	7456 7457	N CA	TYR TYR	211 211		63. 813 64. 634	32. 354 31. 390	1.00 21.78	В	N
ATOM	7458	CB	TYR	211		65. 681	32. 175	1. 00 20. 95 1. 00 18. 35	B B	C
ATOM	7459	CG	TYR	211		66. 566	31.411	1.00 15.38	В	C C C C C C
ATOM	7460		TYR	211		66.086	30. 324	1.00 14.13	В	Č
ATOM	7461		TYR	211		66.879	29.694	1.00 12.47	B	č
ATOM	7462	CD2	TYR	211		67.863	31.846	1.00 11.95	B	Č
ATOM	7463		TYR	211		68.657	31.231	1.00 12.21	В	C
ATOM	7464	CZ	TYR	211		68. 165	30. 156	1.00 13.68	В	
ATOM	7465	OH	TYR	211		68. 977	29. 550	1.00 12.73	В	0
ATOM	7466	C	TYR	211		65. 283	30. 508	1.00 22.11	В	C
ATOM ATOM	7467 7468	O N	TYR SER	211		65. 742	29. 406	1.00 23.55	В	0
ATOM	7469	CA	SER	$\begin{array}{c} 212 \\ 212 \end{array}$		65. 294 65. 877	31. 017 30. 310	1.00 23.17 1.00 22.03	В	N
ATOM	7470	CB	SER	212		66. 055	31. 265	1.00 22.03	B B	C C
ATOM	7471	0G	SER	212		66. 477	30. 567	1.00 24.83	В	0
ATOM	7472	C	SER	212		65.017	29. 141	1.00 22.20	B	č
ATOM	7473	0	SER	212		63.802	29. 256	1.00 22.93	B	Ö
ATOM	7474	N	ALA	213		65.668	28.013	1.00 22.14	В	N
ATOM	7475	CA	ALA	213		65.011	26.812	1.00 19.72	В	C
ATOM	7476	CB	ALA	213		64. 882	25. 803	1.00 19.85	В	C
ATOM	7477	C	ALA	213		65. 942	26. 301	1.00 21.17	В	C
ATOM ATOM	7478 7479	O N	ALA LEU	213		66. 254	25. 109	1.00 20.14	В	0
ATOM	7480	CA	LEU	214 214		66. 409 67. 295	27. 243 26. 961	1.00 21.21 1.00 22.06	В	N
ATOM	7481	CB	LEU	214		68. 697	27. 534	1.00 22.00	B B	C ·
ATOM	7482		LEU	214		69.546	26. 878	1.00 21.02	В	C
ATOM	7483		LEU	214		70.872	27. 603	1.00 21.72	В	Č
ATOM	7484		LEU	214		69. 779	25. 426	1.00 22.01	B	č
ATOM	7485	C	LEU	214		66. 688	27.615	1.00 22.30	B	Č
ATOM	7486	0	LEU	214		66. 131	28.703	1.00 25.61	В	0
ATOM	7487	N	TRP	215		66. 795	26. 957	1.00 21.71	В	· N
ATOM	7488	CA	TRP	215		66. 237	27. 497	1.00 19.34	В	C
ATOM	7489	CB	TRP	215		64. 833	26. 942	1.00 18.71	В	C
ATOM ATOM	7490 7491	CG CD2	TRP	215		63.863	27. 294	1.00 18.43	В	C
ATOM	7491	CE2		215 215		63. 481 62. 536	26. 468 27. 194	1.00 16.56 1.00 14.85	B B	C C C
ATOM	7493	CE3		215		63. 845	25. 186	1.00 14.00	В	r C
ATOM	7494	CD1		215		63. 155	28. 456	1.00 17.01	В	C
ATOM	7495	NE1		215		52. 356	28. 400	1.00 13.49	В	N
ATOM	7496	CZ2		215		61.949	26. 682	1.00 14.75	B	Ċ

					(Continued)
		7. ₄		FIG. 4-154	
ATOM				110. 326 63. 257 24. 675 1. 00 15. 48 B	С
ATOM ATOM	7498	-		109. 599 62. 320 25. 425 1. 00 15. 57 B	C
ATOM	7499 7500			115.110 67.096 27.149 1.00 20.78 B	C
ATOM	7501			115.625 67.034 26.028 1.00 20.20 B	0
ATOM	7502			115.566 67.897 28.108 1.00 20.97 B	N
ATOM	7503			116.727 68.743 27.880 1.00 21.49 B 116.958 69.705 29.048 1.00 22.15 B	C
ATOM	7504			110 000	C
ATOM	7505			114 005 50 000	C
ATOM	7506			115 000 50 510	C
ATOM	7507			110 050 50 50	C
ATOM	7508		216	116. 959 72. 598 27. 452 1. 00 25. 00 B 114. 945 70. 974 29. 994 1. 00 25. 92 B	C C
ATOM	7509	NE1 TRP	216	114. 351 72. 204 29. 844 1. 00 26. 55 B	N N
ATOM	7510		216	114. 815 74. 209 28. 401 1. 00 24. 93 B	C
ATOM	7511	CZ3 TRP	216	116.738 73.887 26.958 1.00 25.52 B	Č
ATOM	7512		216	115.673 74.674 27.435 1.00 24.95 B	č
ATOM	7513		216	117. 982 67. 896 27. 747 1. 00 23. 03 B	č
ATOM	7514		216	118.083 66.816 28.334 1.00 21.32 B	ŏ
ATOM	7515	N SER	217	118.941 68.398 26.975 1.00 25.91 B	Ň
ATOM	7516	CA SER	217	120. 222 67. 723 26. 819 1. 00 26. 96 B	C
ATOM ATOM	7517	CB SER	217	120. 954 68. 223 25. 575 1. 00 28. 77 B	C
ATOM	7518 7519	OG SER C SER	217	121. 212 69. 612 25. 676 1. 00 31. 27 B	0
ATOM	7520	C SER O SER	217 217	120. 976 68. 145 28. 080 1. 00 27. 00 B	C
ATOM	7521	N PRO	218	120. 694 69. 198 28. 656 1. 00 26. 90 B	0
ATOM	7522	CD PRO	218	121. 942 67. 336 28. 523 1. 00 26. 67 B 122. 469 66. 127 27. 867 1. 00 26. 71 B	N
ATOM	7523	CA PRO	218	100 710 07 040 00 707	C
ATOM	7524	CB PRO	218	100 001 00 001	C
ATOM	7525	CG PRO	218	100 005 45 555 00 005	C
ATOM	7526	C PRO	218	123. 385 65. 555 28. 937 1. 00 26. 93 B 123. 005 69. 116 30. 010 1. 00 27. 70 B	C
ATOM	7527	0 PRO	218	122. 487 69. 661 30. 985 1. 00 30. 37 B	C 0
ATOM	7528	n asn	219	123.818 69.770 29.184 1.00 27.72 B	N N
ATOM	7529	CA ASN	219	124. 129 71. 176 29. 435 1. 00 26. 82 B	Č
ATOM	7530	CB ASN	219	125.485 71.562 28.816 1.00 26.61 B	č
ATOM	7531	CG ASN	219	125. 447 71. 640 27. 308 1. 00 27. 23 B	č
ATOM	7532	OD1 ASN	219	124. 376 71. 725 26. 706 1. 00 25. 21 B	Ö
ATOM ATOM	7533	ND2 ASN	219	126. 626 71. 632 26. 690 1. 00 30. 87 B	N
ATOM	7534 7535	C ASN	219	123. 029 72. 133 28. 958 1. 00 27. 38 B	C
ATOM	7536	O ASN N GLY	219	123. 212 73. 351 28. 943 1. 00 29. 12 B	0
ATOM	7537	CA GLY	220	121. 888 71. 575 28. 565 1. 00 26. 98 B	N
ATOM	7538	CA GLY	220 220	120. 765 72. 391 28. 137 1. 00 26. 30 B 120. 823 73. 030 26. 765 1. 00 26. 91 B	C
ATOM	7539	O GLY	220 220	100 000 50 000	C
ATOM	7540	N THR	221	101 000 =0 =1	0
ATOM	7541	CA THR	221	101 000	N
ATOM	7542	CB THR	221	100 000	C
ATOM	7543	OG1 THR	221	123. 052 72. 584 23. 808 1. 00 27. 74 B 124. 213 73. 084 24. 481 1. 00 29. 49 B	C
ATOM		CG2 THR	221	123. 068 73. 089 22. 367 1. 00 26. 25 B	0
ATOM		C THR	221	120. 559 72. 685 23. 730 1. 00 26. 42 B	C C
				CURCULTUTE CHEET (DUI E 2C)	U

					D. T. C	3 4	4 = =			(Cont	tinued)
					FIC	э. 4·	- 155				
ATOM	7546		THR	221	119.862	73. 551	23. 201	1.00 28.29	В	0	
ATOM	7547		PHE	222	120. 305	71.386		1.00 25.34	В	N	
ATOM ATOM	7548 7549		PHE	222	119. 158	70.921	22. 850	1.00 25.13	В	C	
ATOM	7550		PHE PHE	222 222	119.480	69.645	22.069	1.00 25.65	В	C	
ATOM	7551		PHE	222	120. 722 121. 955	69. 723 69. 384		1.00 26.36 1.00 26.35	В	C	
ATOM	7552		PHE	222	120.661	70.111	19.912	1.00 25.81	B B	C C	
ATOM	7553		PHE	222	123. 115	69.425	21. 031	1.00 26.12	В	C	
ATOM	7554		PHE	222	121.815	70. 158	19. 132	1.00 28.19	В	č	
ATOM	7555		PHE	222	123.046	69.814	19.693	1.00 28.46	B	č	
ATOM	7556		PHE	222	117.949	70.618	23.723	1.00 24.55	В	Č	
ATOM	7557		PHE	222	118.066	70. 282	24. 901	1.00 24.38	В	0	
ATOM	7558		LEU	223	116. 780	70. 746	23. 119	1.00 24.19	В	N	
ATOM ATOM	7559 7560	CA CB	LEU LEU	223	115.540	70.442	23. 789	1.00 22.85	В	Č	
ATOM	7561	CG	LEU	$\begin{array}{c} 223 \\ 223 \end{array}$	114.618	71.667 71.340	23. 878	1.00 21.81	В	C	
ATOM	7562		LEU	223	113. 248 113. 469	70.684	24. 503 25. 860	1.00 20.49	В	C	
ATOM	7563		LEU	223	112. 389	72. 587	24.644	1.00 21.10 1.00 18.49	B B	C C	
ATOM	7564	C	LEU	223	114. 885	69.380	22. 934	1.00 23.23	В	C	
ATOM	7565	0	LEU	223	114. 462	69.650	21.808	1.00 22.62	В	Ö	
ATOM	7566	N	ALA	224	114.834	68.162	23. 459	1.00 23.47	В	N	
ATOM	7567	CA	ALA	224	114. 201	67.062	22.753	1.00 23.08	B	Ċ	
ATOM	7568	CB	ALA	224	114. 935	65.776	23.038	1.00 24.27	В	С	
ATOM ATOM	7569	C	ALA	224	112. 761	66.968	23. 248	1.00 23.38	В	C	
ATOM ATOM	7570 7571	O N	ALA TYR	224	112.498	67.111	24. 444	1.00 23.37	В	0	
ATOM	7572	CA	TYR	$\begin{array}{c} 225 \\ 225 \end{array}$	111. 825 110. 423	66.755	22. 328	1.00 23.10	В	N	
ATOM	7573	CB	TYR	225	110. 423	66. 635 67. 997	22. 703 22. 701	1.00 21.31 1.00 18.23	В	C	
ATOM	7574	CG	TYR	225	109. 648	68. 624	21. 332	1.00 18.23	B B	C C C	
ATOM	7575	CD1	TYR	225	110.680	69. 443	20. 849	1.00 16.50	В	C	
ATOM	7576	CE1	TYR	225	110.607	70.017	19. 589	1.00 13.07	В	Č	
ATOM	7577		TYR	225	108. 543	68.399	20.509	1.00 16.18	B	č	
ATOM	7578	CE2	TYR	225	108. 466	68.970	19. 244	1.00 14.89	B	Č	
ATOM	7579	CZ	TYR	225	109. 502	69.777	18.796	1.00 12.68	В	C	
ATOM ATOM	7580 7591	OH	TYR	225	109. 431	70.342	17.553	1.00 14.06	В	0	
ATOM	7581 7582	C 0	TYR TYR	225		65. 712	21.737	1.00 21.55	В	C	
ATOM	7583	N	ALA	225 226		65. 523	20.607	1.00 22.86	В	0	
ATOM	7584	CA	ALA	226		65. 141 64. 235	22. 195 21. 381	1.00 20.96	В	N	
ATOM	7585	CB	ALA	226		62. 980	22. 173	1.00 19.66 1.00 19.19	B B	C	
ATOM	7586	Č	ALA	226		64. 921	20. 962	1.00 19.19	В. В.	C	
ATOM	7587	0	ALA	226		65. 908	21.576	1.00 21.22	В	0	
ATOM	7588	N	GLN	227		64. 410	19. 909	1. 00 16. 70	- B	N	
ATOM	7589	CA	GLN	227	104.659	64.968	19.457	1.00 17.01	\tilde{B}	Ċ	
ATOM	7590	CB	GLN	227		65.709	18.139	1.00 17.47	В	C	
ATOM	7591	CC	GLN	227		66. 300		1.00 18.65	В	С	
ATOM ATOM	7592 7593	CD	GLN	227		66. 788		1.00 18.45	В	C	
ATOM	7594	OE1 NE2	GLN CIN	227 227		66.007		1.00 18.91	В	0	
111 Om	1007	T TO D	ODIT		103.394	68. 090		1.00 19.57	В	N	

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						G. 4-	156			(Continued)
MOTA	7505	C	CI M	997					D	0
ATOM	7595	C	GLN	227	103.651	63. 841	19. 274	1.00 17.21	В	C
ATOM	7596	0 N	GLN	227	103. 931	62. 850	18. 594		В	0
ATOM	7597	N	PHE	228	102. 483	63. 990	19.888	1.00 16.03	В	N C
ATOM	7598	CA	PHE	228 228	101.447	62. 980	19. 768	1.00 17.64	В	C
ATOM ATOM	7599	CB	PHE		100.985	62. 524	21. 158	1.00 14.78	В	C
ATOM	7600 7601	CG	PHE PHE	228 228	102.111	62. 105	22.065	1.00 13.03	В	C
ATOM	7601		PHE	228	102.659	63.003	22. 982	1.00 12.33	В	C
ATOM	7603		PHE	228	102.653	60. 826	21.978	1.00 12.01	В	C
ATOM	7604		PHE	228	103. 732 103. 725	62. 636 60. 450	23. 796 22. 786	1.00 9.77 1.00 11.27	В	C
ATOM	7605	CEZ	PHE	228	103. 723	61.360	23. 698	1.00 11.27	В	C
ATOM	7606	C	PHE	228	104. 267	63. 523	18. 955	1.00 18.96	B B	C C
ATOM	7607	Õ	PHE	228	99. 894	64. 697	19. 064	1.00 18.30	В	0
ATOM	7608	N	ASN	229	99.685	62.657	18. 133	1.00 19.90	В	N
ATOM	7609	CA	ASN	229	98.548	63. 002	17. 285	1.00 20.11	. В	C
ATOM	7610	CB	ASN	229	98. 965	62. 867	15. 819	1.00 20.14	В	C
ATOM	7611	CG	ASN	229	97. 980	63. 488	14. 867	1.00 27.56	В	Č
ATOM	7612		ASN	229	96. 795	63.610	15. 174	1.00 21.50	В	Ö
ATOM	7613		ASN	229	98. 467	63. 871	13. 692	1.00 30.76	В	N
ATOM	7614	C	ASN	229	97. 435	61.995	17.609	1.00 21.10	В	Č
ATOM	7615	Õ,	4000	229	97. 550	60.816	17. 283		В	ŏ
ATOM	7616	Ň	ASP	230	96. 369	62. 444	18. 260	1.00 22.16	B	N
ATOM	7617	CA	ASP	230	95. 277	61.534	18.608	1.00 24.31	B	Ċ
ATOM	7618	CB	ASP	230	94.877	61. 683	20.079	1.00 23.86	B	č
ATOM	7619	CG	ASP	230	95.999	61.332	21.027	1.00 25.25	B	č
ATOM	7620	0D1	ASP	230	95.701	60.914	22.159	1.00 27.89	B	Ö
ATOM	7621	0D2	ASP	230	97.180	61.485	20.656	1.00 27.78	B	Ö .
ATOM	7622	C	ASP	230	94.056	61.776	17.740	1.00 24.83	В	Č
ATOM	7623	0	ASP	230	92.927	61.496	18.148	1.00 24.00	В	0
ATOM	7624	N	THR	231	94.297	62.284	16.536	1.00 25.37	В	N
ATOM	7625	CA	THR	231	93.229	62.582	15. 593	1.00 26.24	В	C
ATOM	7626	CB	THR	231	93.802	62.868	14. 193	1.00 25.71	В	C
ATOM	7627		THR	231	94. 439	64. 151	14. 194	1.00 26.78	В	0
ATOM	7628		THR	231	92. 702	62.851	13. 150	1.00 23.72	В	C
ATOM	7629	C	THR	231	92.148	61.510	15.467	1.00 27.04	В	C
ATOM	7630	0	THR	231	90.964	61.815	15.604	1.00 29.05	В	0
ATOM	7631	N	GLU	232	92. 545	60. 265	15. 211	1.00 27.00	В	N
ATOM	7632	CA	GLU	232	91.574	59. 183	15.038	1.00 26.30	В	C
ATOM	7633	CB	GLU	232	92.017	58. 286	13.877	1.00 29.71	В	C C C
ATOM	7634	CG	GLU	232	92. 177	59.036	12.563	1.00 36.71	В	C
ATOM	7635	CD	GLU	232	92. 971	58. 253	11.519	1.00 39.94	В	C
ATOM	7636		GLU	232	92. 434	57. 273	10.943	1.00 41.61	В	. 0
ATOM	7637		GLU	232	94. 142	58. 623	11. 286	1.00 39.28	В	0
ATOM	7638 7639	C	GLU	232	91.320	58. 328	16. 282	1.00 23.78	В	C
ATOM ATOM	7640	0 N	GLU	232	90. 683	57. 280	16. 208	1.00 23.18	В	0
ATOM	7641	CA	VAL VAL	233 233	91.823	58. 763	17. 427	1.00 21.91	В	N
ATOM	7642	CB	VAL	233 233	91.608	58.010	18.652	1.00 20.18	В	C
ATOM	7643	CG1		233 233	92.651	58.375	19. 727	1.00 20.26	B B	C C
INTOIL	. 0 10	201	TIL	400	92. 352	57.627	21.016	1.00 18.23	מ	U

					FIC	3. 4·	- 157			(Continued)
ATOM	7644		2 VAI		94. 050	58. 032	19. 223	1.00 18.80	В	Ç
ATOM ATOM	7645 7646		VAL		90. 218	58. 339		1.00 18.04	В	C
ATOM	7647		VAL PRO		89. 886	59.507		1.00 19.49	В	0
ATOM	7648				89. 383 89. 633	57.315		1.00 16.04	В	N
ATOM	7649				88. 025	55. 876 57. 544		1.00 14.37	В	. C
ATOM	7650				87. 461	56. 133		1.00 15.33 1.00 13.91	В	C
ATOM	7651	CG			88. 247	55. 363		1.00 13.91	В	C C
ATOM	7652		PRO		88. 048	58. 275		1.00 12.65	B B	C
ATOM	7653		PRO		89. 043	58. 242	21. 950	1.00 14.43	В	Õ
ATOM	7654		LEU		86. 941	58. 927	21.547	1.00 14.92	В	N N
ATOM	7655				86. 831	59.676	22. 791	1.00 13.91	В	Č
ATOM	7656	CB	LEU		86. 131	61.005	22. 536	1.00 14.93	В	č
ATOM	7657	CG			86.627	61.937	21.434	1.00 16.83	В	č
ATOM	7658	CD	1 LEU		85. 581	63.030	21.198	1.00 17.90	В	č
ATOM	7659	CD	2 LEU	235	87.963	62.534	21.833	1.00 14.85	B	Č
ATOM	7660	C	LEU		85.998	58.911	23.803	1.00 12.70	B	Č
ATOM	7661	0	LEU		84. 941	58. 385	23.456	1.00 13.27	В	0
ATOM	7662	N	ILE		86.468	58. 801	25.039	1.00 10.71	В	N
ATOM	7663	CA	ILE		85.618	58. 165	26.037	1.00 10.96	В	С
ATOM	7664	CB	ILE		86. 385	57.630	27. 283	1.00 9.70	В	C
ATOM	7665		ILE ILE		87. 316	58. 692	27.859	1.00 10.05	В	С
ATOM ATOM	7666		ILE	236	85. 386	57. 246	28.371	1.00 7.51	В	С
ATOM	7667 7668		ILE	236	84. 465	56. 100	28.002	1.00 9.77	В	Č
ATOM	7669	C 0	ILE ILE	$\frac{236}{236}$	84.774	59.369	26.456	1.00 12.91	В	Č
ATOM	7670	N	GLU	$\begin{array}{c} 236 \\ 237 \end{array}$	85. 277	60.500	26.486	1.00 13.64	В	0
ATOM	7671	CA	GLU	237	83. 497	59. 156	26.741	1.00 13.69	B .	N
ATOM	7672	CB	GLU	237	82. 651 81. 657	60. 267	27. 150	1.00 14.30	В	C
ATOM	7673	CG	GLU	237	82. 307	60. 643 60. 993	26. 041 24. 708	1.00 15.93	В	C -
ATOM	7674	CD	GLU	237	81.311	61.541	23. 682	1.00 20.06 1.00 24.67	В	C
ATOM	7675		GLU	237	80. 133	61.125	23. 713	1.00 24.07	В	C .
ATOM	7676		GLU	237	81.706	62. 377	22. 832	1.00 27.11	B B	0 0
ATOM	7677	C	GLU	237	81. 902	59. 898		1.00 23.11	В	C
ATOM	7678	0	GLU	237	81.473	58. 759	28. 569	1.00 12.02	В	0
ATOM	7679	N	TYR	238	81.768	60.860	29.310	1.00 12.67	В	N
ATOM	7680	CA	TYR	238	81.044	60.630	30.550	1.00 13.08	B	Č
ATOM	7681	CB	TYR	238	81.903	59.816	31.534	1.00 11.88	B	Č
ATOM	7682	CG	TYR	238	83. 201	60.458	31.954	1.00 15.20	B	Č
ATOM	7683	CD1		238	83. 250	61.347	33.026	1.00 15.46	$\tilde{\mathbf{B}}$	č
ATOM	7684		TYR	238	84. 458	61.920	33. 430	1.00 15.78	В	Č
ATOM	7685		TYR	238		60.160	31. 291	1.00 14.07	В	Ċ
ATOM	7686		TYR	238		60. 727	31.683	1.00 14.24	В	Č
ATOM	7687	CZ	TYR	238		61.606	32. 751	1.00 13.94	В	С
ATOM	7688	OH	TYR	238		62. 173	33. 129	1.00 12.45	В	0
ATOM	7689	C	TYR	238		61.944	31. 163	1.00 13.53	В	C
ATOM	7690	0 N	TYR	238		63.008	30. 832	1.00 14.88	В	0
ATOM ATOM	7691 7692	N CA	SER	239		61.865	32. 042	1.00 14.64	В	N
VION	(034	CA	SER	239	79.040	63.047	32. 684	1.00 13.89	В	C

						(Continued)
			,		FIG. 4-158	(Continuou)
ATOM	7693		SER	239	77. 597 62. 783 33. 085 1. 00 13. 29 B	C
ATOM	7694		SER	239	76. 800 62. 496 31. 961 1. 00 19. 37 B	0
ATOM	7695		SER	239	79. 775 63. 547 33. 915 1. 00 14. 65 B	Č
ATOM	7696		SER	239	80. 361 62. 775 34. 673 1. 00 15. 52 B	0
ATOM	7697		PHE	240	79. 737 64. 860 34. 100 1. 00 14. 89 B	N
ATOM	7698		PHE	240	80. 313 65. 493 35. 276 1. 00 15. 60 B	Ĉ
ATOM	7699		PHE	240	81. 543 66. 325 34. 932 1. 00 17. 00 B	Č
ATOM	7700		PHE	240	82. 422 66. 591 36. 112 1. 00 14. 96 B	C C C C C C
ATOM	7701		PHE	240	83. 325 65. 629 36. 547 1. 00 15. 66 B	Č
ATOM	7702		PHE	240	82. 312 67. 781 36. 822 1. 00 14. 41 B	Č
ATOM	7703		PHE	240	84. 108 65. 846 37. 675 1. 00 13. 32 B	Č
ATOM	7704		PHE	240	83. 087 68. 009 37. 950 1. 00 12. 45 B	Č
ATOM	7705		PHE	240	83. 988 67. 039 38. 379 1. 00 11. 23 B	Č
ATOM	7706		PHE	240	79. 184 66. 403 35. 758 1. 00 15. 75 B	Č
ATOM	7707		PHE	240	78. 671 67. 232 34. 995 1. 00 14. 05 B	Ö
ATOM	7708	N	TYR	241	78. 785 66. 231 37. 013 1. 00 15. 13 B	N
ATOM	7709	CA	TYR	241	77. 683 67. 002 37. 567 1. 00 14. 92 B	Ċ
ATOM	7710	CB	TYR	241	76. 912 66. 125 38. 545 1. 00 13. 15 B	Č
ATOM	7711	CG	TYR	241	76. 480 64. 848 37. 880 1. 00 12. 77 B	č
ATOM	7712		TYR	241	75. 393 64. 832 37. 007 1. 00 11. 36 B	č
ATOM	7713		TYR	241	75. 051 63. 678 36. 304 1. 00 12. 47 B	C C C
ATOM	7714		TYR	241	77. 215 63. 674 38. 041 1. 00 12. 85 B	č
ATOM	7715		TYR	241	76. 883 62. 512 37. 342 1. 00 12. 55 B	č
ATOM	7716	CZ	TYR	241	75. 801 62. 523 36. 472 1. 00 12. 41 B	č
ATOM	7717	OH	TYR	241	75. 489 61. 395 35. 748 1. 00 12. 90 B	Ö
ATOM	7718	C	TYR	241	78. 100 68. 299 38. 208 1. 00 15. 24 B	Č
ATOM	7719	0	TYR	241	77. 311 69. 239 38. 263 1. 00 17. 04 B	Ö
ATOM	7720	N	SER	242	79. 337 68. 353 38. 694 1. 00 16. 92 B	Ň
ATOM	7721	CA	SER	242	79. 864 69. 570 39. 305 1. 00 16. 89 B	Ċ
ATOM	7722	CB	SER	242	79. 816 70. 707 38. 280 1. 00 15. 48 B	Č
ATOM	7723	0G	SER	242	80. 439 71. 870 38. 782 1. 00 18. 12 B	0
ATOM	7724	C	SER	242	79.078 69.963 40.548 1.00 16.70 B	Č
ATOM	7725	0	SER	242	78. 438 69. 121 41. 171 1. 00 18. 07 B	0
ATOM	7726	N	ASP	243	79. 136 71. 241 40. 912 1. 00 17. 57 B	N
ATOM	7727	CA	ASP	243	78. 405 71. 728 42. 075 1. 00 19. 72 B	C
ATOM	7728	CB	ASP	243	78. 846 73. 142 42. 442 1. 00 23. 43 B	Ċ
ATOM	7729		ASP	243	80. 275 73. 188 42. 950 1. 00 28. 70 B	Č
ATOM	7730	OD1		243	80. 646 72. 307 43. 765 1. 00 29. 62 B	0
ATOM	7731	OD2		243	81. 021 74. 106 42. 542 1. 00 29. 69 B	0
ATOM	7732	C	ASP	243	76.917 71.708 41.772 1.00 20.24 B	C
ATOM	7733		ASP	243	76.508 71.777 40.609 1.00 20.38 B	0
ATOM	7734		GLU	244	76. 104 71. 624 42. 818 1. 00 19. 25 B	N
ATOM	7735		GLU	244	74.668 71.545 42.630 1.00 19.29 B	Ċ
ATOM	7736		GLU	244	73.966 71.376 43.988 1.00 19.46 B	Ċ
ATOM	7737		GLU	244	73. 283 72. 609 44. 533 1. 00 23. 65 B	Č
ATOM	7738		GLU	244	72. 567 72. 334 45. 847 1. 00 26. 30 B	Č
ATOM	7739	0E1		244	73. 225 71. 856 46. 797 1. 00 28. 64 B	0
ATOM	7740	0E2		244	71.349 72.595 45.934 1.00 27.72 B	0
ATOM	7741	C	GLU	244	74. 086 72. 720 41. 850 1. 00 18. 30 B	Č
					SUBSTITUTE SHEET (PUI E 26)	

ATOM 7742 0 GLU 244 72.958 72.647 41.355 1.00 19.81 B 0 ATOM 7743 N SER 245 74.861 73.785 41.702 1.00 15.52 B N ATOM 7744 CA SER 245 74.381 74.958 40.986 1.00 11.95 B C ATOM 7745 CB SER 245 75.157 76.196 41.425 1.00 11.90 B C ATOM 7746 0G SER 245 76.473 76.162 40.915 1.00 17.74 B 0 ATOM 7747 C SER 245 74.459 74.821 39.470 1.00 9.32 B C ATOM 7748 0 SER 245 73.883 75.625 38.752 1.00 10.56 B 0 ATOM 7749 N LEU 246 75.167 73.819 38.968 1.00 8.50 B N ATOM 7750 CA LEU 246 75.252 73.647 37.518 1.00 8.56 B C ATOM 7751 CB LEU 246 76.481 72.812 37.145 1.00 8.57 B C ATOM 7753 CD1 LEU 246 76.770 72.639 35.644 1.00 11.81 B C ATOM 7754 CD2 LEU 246 77.074 73.984 35.008 1.00 5.99 B C ATOM 7755 C LEU 246 77.949 71.694 35.449 1.00 10.70 B C ATOM 7756 0 LEU 246 73.971 72.944 37.070 1.00 10.18 B C		FIG. 4-159	(Continued)
ATOM 7757 N GLN 247 73.094 73.685 36.393 1.00 12.01 B N 7758 CA GLN 247 71.815 73.144 35.938 1.00 12.01 B N 7759 CB GLN 247 70.995 74.230 35.245 1.00 12.00 B C 7759 CB GLN 247 69.584 73.806 34.984 1.00 14.88 B C 7750 CB GLN 247 68.727 74.978 34.446 1.00 14.88 B C 7750 CB GLN 247 69.584 73.806 34.984 1.00 14.88 B C 7750 CB GLN 247 69.584 73.806 34.986 1.00 13.91 B N 7759 CB GLN 247 69.152 75.069 34.986 1.00 13.91 B N 7759 CB GLN 247 69.152 75.069 34.986 1.00 13.91 B N 7759 CB GLN 247 71.974 71.942 35.022 1.00 12.63 B C 7750 M 7766 N MEZ GLN 247 71.974 71.942 35.022 1.00 12.63 B C 7750 M 7766 N TYR 248 72.793 72.074 33.987 1.00 13.50 B O 7750 M 7766 N TYR 248 73.022 70.949 33.089 1.00 13.50 B O 7750 M 7766 CG TYR 248 73.022 70.949 33.089 1.00 13.90 B C 7750 M 7760	ATOM 7743 N SER 245 ATOM 7744 CA SER 245 ATOM 7745 CB SER 245 ATOM 7746 OG SER 245 ATOM 7747 C SER 245 ATOM 7747 C SER 245 ATOM 7748 O SER 245 ATOM 7749 N LEU 246 ATOM 7750 CA LEU 246 ATOM 7751 CB LEU 246 ATOM 7752 CG LEU 246 ATOM 7753 CD1 LEU 246 ATOM 7755 C LEU 246 ATOM 7756 O LEU 246 ATOM 7756 O LEU 246 ATOM 7757 N GLN 247 ATOM 7757 N GLN 247 ATOM 7758 CA GLN 247 ATOM 7759 CB GLN 247 ATOM 7760 CG GLN 247 ATOM 7760 CG GLN 247 ATOM 7761 CD GLN 247 ATOM 7760 CG GLN 247 ATOM 7760 CG GLN 247 ATOM 7760 CG GLN 247 ATOM 7761 CD GLN 247 ATOM 7762 OE1 GLN 247 ATOM 7763 NE2 GLN 247 ATOM 7766 N TYR 248 ATOM 7766 N TYR 248 ATOM 7767 CA TYR 248 ATOM 7768 CB TYR 248 ATOM 7769 CG TYR 248 ATOM 7769 CG TYR 248 ATOM 7770 CD1 TYR 248 ATOM 7770 CD1 TYR 248 ATOM 7771 CE1 TYR 248 ATOM 7770 CD1 TYR 248 ATOM 7770 CD2 TYR 248 ATOM 7770 CD2 TYR 248 ATOM 7770 CD2 TYR 248 ATOM 7771 CE1 TYR 248 ATOM 7770 CD TYR 248 ATOM 7771 CE TYR 248 ATOM 7773 CE TYR 248 ATOM 7773 CE TYR 248 ATOM 7776 C TYR 248 ATOM 7777 C TYR 248 ATOM 7778 CE TYR 248 A	72. 958 72. 647 41. 355 1. 00 19. 81 74. 861 73. 785 41. 702 1. 00 15. 52 74. 381 74. 958 40. 986 1. 00 11. 95 75. 157 76. 196 41. 425 1. 00 11. 90 76. 473 76. 162 40. 915 1. 00 17. 74 74. 459 74. 821 39. 470 1. 00 9. 32 73. 883 75. 625 38. 752 1. 00 10. 56 75. 167 73. 819 38. 968 1. 00 8. 56 76. 481 72. 812 37. 145 1. 00 8. 57 76. 70 72. 639 35. 644 1. 00 11. 81 77. 074 73. 984 35. 008 1. 00 5. 99 77. 949 71. 694 35. 449 1. 00 10. 70 73. 971 72. 944 37. 070 1. 00 10. 18 73. 722 71. 758 37. 349 1. 00 12. 01 71. 815 73. 144 35. 938 1. 00 12. 01 71. 815 73. 144 35. 938 1. 00 12. 01 71. 87 74. 978	B B B B B B B B B B B B B B B B B B B

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, 1,7%					FIG	. 4 -	160			(Continued)
ATOM ATOM	7791 7792	NZ C	LYS LYS	250		70. 465	31.442	1.00 26.19	В	N
ATOM	7793	0	LYS	250 250		67.313	31.040 31.867	1.00 17.64	В	C
ATOM	7794	N	THR	250 251		66. 409 67. 160	29. 750	1.00 20.20 1.00 15.06	B B	O N
ATOM	7795	CA	THR	251		65. 905	29. 234	1.00 13.00	В	C
ATOM	7796	CB	THR	251		65. 537	27. 896	1.00 14.31	В	Č
ATOM	7797		THR	251		65. 144	28. 128	1.00 14.97	В	ŏ
ATOM	7798		THR	251		64. 389	27. 227	1.00 13.23	В	Č
ATOM	7799	C	THR	251		66.016	29. 015	1.00 15.66	В	č
ATOM	7800	Ŏ	THR	251		66. 831	28. 227	1.00 18.88	B	ŏ
ATOM	7801	N	VAL	252		65. 194	29. 720	1.00 15.28	B	Ň
ATOM	7802	CA	VAL	252		65. 195	29.578	1.00 15.13	В	C
ATOM	7803	CB	VAL	252		64.717	30.882	1.00 13.64	В	С
ATOM	7804		VAL	252		64. 580	30.706	1.00 10.22	В	C
ATOM	7805		VAL	252		65. 701	31. 991	1.00 11.83	В	C
ATOM	7806	C	VAL	252		64. 264	28. 422	1.00 17.21	В	C
ATOM	7807	0	VAL	252		63. 173	28. 304	1.00 17.34	В	0
ATOM	7808	N ₋	ARG	253		64.710	27. 557	1.00 18.91	В	N
ATOM	7809	CA	ARG	253		63. 922	26. 403	1.00 20.46	В	C
ATOM	7810	CB	ARG	253		64. 560	25. 113	1.00 22.21	В	C
ATOM	7811	CC	ARG	253		64. 137	24. 755	1.00 26.72	В	C
ATOM ATOM	7812 7813	CD NE	ARG ARG	253 253		64. 920	23. 578	1.00 28.87	В	C
ATOM	7814	CZ	ARG	253		66. 132	24.033	1.00 36.20	В	N C
ATOM	7815		ARG	$\frac{253}{253}$		66. 221 65. 164	24. 278 24. 099	1.00 38.47 1.00 39.84	B B	C
ATOM	7816		ARG	253		67. 360	24. 727	1.00 39.84	В	N N
ATOM	7817	C	ARG	253		63.863	26. 389	1.00 37.37	В	C
ATOM	7818	ŏ	ARG	253		64. 886	26. 246	1.00 21.87	В	ŏ
ATOM	7819	N	VAL	254		62.656	26.538	1.00 18.34	В	Ň
ATOM	7820	CA	VAL	254		62. 434	26. 594	1.00 15.15	В	
ATOM	7821	CB	VAL	254		61.924	27. 994	1.00 16.16	B	C C C C
ATOM	7822	CG1		254		61.759	28.081	1.00 15.18	B	Č
ATOM	7823	CG2		254	88. 736	62.868	29.065	1.00 16.46	В	С
ATOM	7824	C	VAL	254		61.397	25.585	1.00 14.67	В	С
ATOM	7825		VAL		88. 806			1.00 14.87	В	0
ATOM	7826	N	PRO	255		61.757	24. 726	1.00 13.62	В	N
ATOM	7827	CD	PRO	255		63. 081	24. 472	1.00 12.90	В	N C C C C
ATOM	7828	CA	PRO	255		60. 777	23. 746	1.00 12.62	В	Ċ
ATOM	7829	CB	PRO	255		51.566	22. 933	1.00 11.40	В	C
ATOM	7830	CG	PRO	255		62. 969	23. 013	1.00 11.65	В	C
ATOM ATOM	7831 7832	C 0	PRO PRO	255		59. 645	24. 553	1.00 12.46	В	C
ATOM	7833	N	TYR	255 256		59. 831	25. 282	1.00 13.25	В	0
ATOM	7834	CA	TYR	256		58. 469 57. 306	24. 414 25. 161	1.00 12.53 1.00 12.05	B B	N C
ATOM	7835	CB	TYR	256 256		57. 205	26. 398	1.00 12.05	В	C C
ATOM	7836	CG	TYR	256		56. 082	27. 360	1.00 12.42	В	C
ATOM	7837		TYR	256		56. 355	28. 662	1.00 14.33	В	C
ATOM	7838	CE1		256		55. 337	29. 596	1.00 10.44	В	C
ATOM	7839	CD2		256		54. 752	27. 010	1.00 15.31	B	č

					FIG. 4-161		(Continued)
ATOM ATOM	7840 7841	CZ		256 256	90. 548 53. 724 27. 941 1. 00 16. 91 90. 949 54. 030 29. 232 1. 00 16. 54	B B	C C
ATOM ATOM	7842 7843		TYR TYR	$\begin{array}{c} 256 \\ 256 \end{array}$	91.068 53.042 30.176 1.00 17.03	В	0
ATOM	7844		TYR	256 256	91. 040 56. 094 24. 263 1. 00 11. 63 89. 923 55. 765 23. 870 1. 00 13. 76	B B	C
ATOM	7845		PRO	257	92.141 55.415 23.924 1.00 10.78	В	O N
ATOM	7846			257	93. 535 55. 786 24. 231 1. 00 9. 21	В	Č
ATOM	7847			257	92. 098 54. 229 23. 068 1. 00 9. 97	В	Č
ATOM ATOM	7848			257	93. 473 54. 233 22. 438 1. 00 8. 95	В	C
ATOM	7849 7850		PRO PRO	$\begin{array}{c} 257 \\ 257 \end{array}$	94.326 54.657 23.606 1.00 8.91	B	C
ATOM	7851	0	PRO	257	91. 859 52. 949 23. 869 1. 00 11. 12 92. 694 52. 556 24. 681 1. 00 9. 90	B	C
ATOM	7852	Ň	LYS	258	90. 723 52. 300 23. 648 1. 00 11. 97	B B	O N
ATOM	7853	CA	LYS	258	90. 444 51. 057 24. 353 1. 00 13. 52	В	C
ATOM	7854	CB	LYS	258	88. 930 50. 855 24. 492 1. 00 15. 66	B	č
ATOM	7855	CG	LYS	258	88. 305 51. 808 25. 522 1. 00 14. 41	В	Ċ
ATOM ATOM	7856 7857	CD	LYS	258		В	C
ATOM	7858	CE NZ	LYS LYS	258 258		В	C
ATOM	7859	C	LYS	258		B	N
ATOM	7860	Ŏ	LYS	258	01 500 50 100 00 100	B B	C 0
ATOM	7861	N	ALA	259	01 007 10 500 01 175	В	N N
ATOM	7862	ÇA	ALA	259	91. 874 47. 627 23. 515 1. 00 14. 83	B	Ċ
ATOM	7863	CB	ALA	259	91. 564 46. 356 24. 261 1. 00 14. 32	B	Č
ATOM ATOM	7864 7865	C	ALA	259		В	C
ATOM	7866	O N	ALA GLY	259 260		В	0
ATOM	7867	CA	GLY	260		B	N
ATOM	7868	C	GLY	260	01 011 10 700	B B	C C
ATOM	7869	0	GLY	260	01 701 40 400 15 55	В	0
ATOM	7870	N	ALA	261	01 505 45 600	B	N
ATOM	7871	CA	ALA	261	91. 198 50. 851 18. 983 1. 00 14. 89	B	Ĉ
ATOM ATOM	7872 7873	CB C	ALA	261	90. 557 51. 830 19. 963 1. 00 13. 58	В	С
ATOM	7874	Ö	ALA ALA	261 261	00 400 50 000 40 000	В	C .
ATOM	7875	N	VAL	262	00 105 50 400 15 400	В	0
ATOM	7876	CA	VAL	262	00 100 50 001	B B	N C
ATOM	7877	CB	VAL	262	00 014 54 054	В	C
ATOM	7878		VAL	262	93.717 55.252 15.383 1.00 13.59	B	č
ATOM	7879		VAL	262	91. 970 53. 596 14. 820 1. 00 10. 82 I	В	č
ATOM ATOM	7880	C	VAL	262		В	С
ATOM	7881 7882	O N	VAL ASN	262 263		В	0
ATOM	7883	CA	ASN	263 263	95. 275 53. 856 18. 128 1. 00 16. 87 96. 190 54. 493 19. 068 1. 00 17. 45		N
ATOM	7884	CB	ASN	263	96. 190 54. 493 19. 068 1. 00 17. 45 97. 406 53. 595 19. 292 1. 00 17. 58		C
ATOM	7885	CG	ASN	263	97. 230 52. 629 20. 437 1. 00 20. 08		C C
ATOM	7886.		ASN	263	97. 919 51. 606 20. 500 1. 00 19. 88 B		0
ATOM	7887		ASN	263	96. 329 52. 950 21. 365 1. 00 18. 44 B		N
ATOM	7888	C	ASN	263	96. 706 55. 827 18. 533 1. 00 18. 01 B		Č

	•		•		F. I	G. 4	-162	;		(Continued)
ATOM ATOM	7889 7890	N	ASN PRO	263 264	96. 578 97. 288	56.646			B B	0 N
ATOM	7891	CD		264	97. 357				В	C
ATOM	7892			264	97. 819				В	C
ATOM ATOM	7893 7894			264	98. 089			1.00 14.78	В	C
ATOM	7895	C	PRO	$\begin{array}{c} 264 \\ 264 \end{array}$	98. 411 99. 105				В	C
ATOM	7896	0	PRO	$\begin{array}{c} 204 \\ 264 \end{array}$	99. 669				В	C
ATOM	7897	N	THR	265	99. 560			1.00 15.27 1.00 16.21	B B	0 N
ATOM	7898	CA		265	100. 796			1.00 10.21	В	N C
ATOM	7899	CB		265	100.647			1.00 15.20	В	Č
ATOM	7900	OG.		265	100.081	59. 983		1.00 17.05	В	ŏ
ATOM	7901	CG	2 THR	265	99. 747	57.687		1.00 10.60	·B	č
ATOM	7902	C	THR	265	101.818	59. 211	17: 279	1.00 16.13	B	Č
ATOM	7903	0	THR	265	101.454			1.00 16.83	В	0
ATOM	7904	Ņ	VAL	266	103.095	58. 971	17.030	1.00 17.64	В	N
ATOM ATOM	7905	CA	VAL	266	104. 118	59. 781	17.667	1.00 17.49	В	C
ATOM	7906 7907	CB	VAL VAL	266 266	104.626	59.060	18. 930	1.00 15.28	В	C
ATOM	7908		VAL VAL	266	105. 224 105. 642	57. 714 59. 921	18.538	1.00 12.10	В	C
ATOM	7909	C	VAL	266	105. 042	60. 112	19.666 16.769	1.00 12.62	В	C
ATOM	7910	ŏ	VAL	266	105. 693	59. 331	15. 893	1.00 19.23 1.00 18.24	B B	C
ATOM	7911	Ň	LYS	267	105. 889	61. 287	17.003	1.00 18.24	В	O N
ATOM	7912	CA	LYS	267	107.058	61.756	16. 272	1.00 19.42	В	C
ATOM	7913	CB	LYS	267	106.678	62.855	15. 291	1.00 19.76	В	Č
ATOM	7914	CG	LYS	267	105. 786	62.413	14.168	1.00 21.59	B	č
ATOM	7915	CD	LYS	267	105.452	63.605	13. 291	1.00 23.15	В	Č
ATOM	7916	CE	LYS	267	104. 593	63. 205	12.119	1.00 23.47	В	C
ATOM	7917	NZ	LYS	267	104. 225	64. 402	11. 334	1.00 27.20	В	N
ATOM ATOM	7918 7919	C 0	LYS	267	108.032	62.334	17. 288	1.00 19.59	В	C
ATOM	7920	N	LYS PHE	267 268	107.618	62.826	18.336	1.00 20.86	В	0
ATOM	7921	CA	PHE	268	109. 322 110. 325	62. 275 62. 818	16.984	1.00 19.32	В	N
ATOM	7922	CB	PHE	268	111.350	61.757	17. 882 18. 259	1.00 18.94 1.00 17.47	В	C
ATOM	7923	CG	PHE	268	112. 186	62. 131	19. 444	1.00 17.47	В	C
ATOM	7924		PHE	268	111.601	62. 290	20. 692	1.00 16.21	B B	C C
ATOM	7925		PHE	268	113.555	62.327	19.313	1.00 16.35	В	C
ATOM	7926		PHE	268	112.368	62.639	21.797	1.00 18.80	B	Č
ATOM	7927		PHE	268	114. 332	62.674	20.405	1.00 17.68	B	č
ATOM	7928	CZ	PHE	268	113. 737	62.832	21.655	1.00 18.66	B	Č
ATOM	7929	Ç	PHE	268	111.016	63.979	17. 192	1.00 20.34	В	Ċ
ATOM	7930	0	PHE	268	111.114	64.016	15.968	1.00 21.73	В	0
ATOM ATOM	7931 7932	N Ca	PHE	269	111.491	64. 931	17. 981	1.00 20.76	В	N
ATOM	7932 7933	CA CB	PHE PHE	269 269	112.152	66. 105	17. 435	1.00 20.74	В	C
ATOM	7934	CG	PHE	269 269	111.141 110.070	67. 239	17. 222	1.00 19.80	В	C
ATOM	7935		PHE	269	110.070	66. 937 67. 019	16. 216	1.00 21.88	В	C
ATOM	7936		PHE	269	10. 332	66.605	14. 853 16. 631	1.00 22.75 1.00 23.20	В	C
ATOM	7937		PHE	269	109. 326	66. 781	13. 912	1.00 23.20	B B	C
						_		·		-

FIG. 4 - 163 ATOM 7938 CE2 PHE 269 107.771 66.364 15.700 1.00 23.06 B C 108.044 66.454 14.337 1.00 22.44 B C	
ATOM 7938 CE2 PHE 269 107.771 66.364 15.100 1.00 22.44 B C	
ATOM 7940 C PHE 269 113. 209 66. 606 18. 402 1. 00 21. 66 B C ATOM 7941 O PHE 269 113. 209 66. 606 18. 402 1. 00 21. 66 B C ATOM 7941 O PHE 269 113. 127 66. 376 19. 613 1. 00 21. 27 B O ATOM 7942 N VAL 270 114. 195 67. 305 17. 858 1. 00 23. 26 B C ATOM 7944 C B VAL 270 116. 529 67. 896 18. 667 1. 00 23. 26 B C ATOM 7944 C GC VAL 270 116. 529 67. 896 18. 667 1. 00 23. 20 B C ATOM 7945 CG1 VAL 270 116. 529 67. 896 18. 667 1. 00 23. 10 B C ATOM 7946 CG2 VAL 270 116. 529 67. 896 18. 895 1. 00 23. 00 B C ATOM 7947 C VAL 270 116. 600 69. 460 16. 880 1. 00 26. 90 B O ATOM 7947 C VAL 270 115. 600 69. 460 16. 880 1. 00 26. 90 B O ATOM 7949 N VAL 271 115. 561 70. 278 18. 973 1. 00 26. 96 B N ATOM 7950 CA VAL 271 115. 591 70. 278 18. 973 1. 00 26. 96 B N ATOM 7950 CA VAL 271 114. 516 72. 514 18. 714 1. 00 28. 95 B C ATOM 7952 CG1 VAL 271 114. 516 72. 514 18. 714 1. 00 28. 95 B C ATOM 7955 CG VAL 271 114. 569 73. 915 18. 186 1. 00 27. 45 B C ATOM 7955 CG VAL 271 114. 696 72. 563 20. 177 1. 00 28. 40 B C ATOM 7955 CG VAL 271 114. 696 72. 563 20. 177 1. 00 28. 40 B C ATOM 7955 CG VAL 271 117. 094 71. 935 0. 50. 50 ATOM 7955 CG ASN 272 119. 951 74. 656 18. 378 1. 00 27. 39 B C ATOM 7956 CB ASN 272 119. 951 74. 656 18. 378 1. 00 27. 39 B C ATOM 7956 CB ASN 272 119. 951 74. 656 18. 378 1. 00 27. 45 B C ATOM 7960 ODI ASN 272 121. 197 74. 672 19. 031 1. 00 28. 35 B C ATOM 7960 ODI ASN 272 121. 197 74. 672 19. 031 1. 00 27. 45 B C ATOM 7960 CA SN 272 118. 347 75. 104 19. 972 1. 00 28. 35 B C ATOM 7966 CB THR 273 118. 898 77. 516 1. 997 1. 00 28. 35 B C ATOM 7960 ODI ASN 272 121. 197 74. 672 19. 031 1. 00 27. 45 B C ATOM 7960 ODI ASN 272 121. 197 74. 672 19. 031 1. 00 27. 45 B C ATOM 7960 CA SR 272 118. 347 75. 104 19. 972 1. 00 27. 45 B C ATOM 7960 ODI ASN 272 121. 197 74. 672 19. 031 1. 00 28. 35 B C ATOM 7960 ODI ASN 272 121. 197 74. 672 19. 031 1. 00 27. 45 B C ATOM 7960 ODI ASN 272 121. 197 74. 672 19. 031 1. 00 27. 45 B C ATOM 7960 ODI ASN 272 121. 197 74. 672 19. 00 18. 90 10 10 10 10 10 10 10 10 10 10 10 10 10	

	FIG. 4-164	(Continued)
ATOM 7987 CB LEU 276 ATOM 7988 CG LEU 276 ATOM 7989 CD1 LEU 276 ATOM 7990 CD2 LEU 276 ATOM 7991 C LEU 276 ATOM 7991 C LEU 276 ATOM 7992 O LEU 276 ATOM 7992 O LEU 276 ATOM 7993 N SER 277 ATOM 7994 CA SER 277 ATOM 7995 CB SER 277 ATOM 7996 OG SER 277 ATOM 7997 C SER 277 ATOM 7998 O SER 277 ATOM 7999 N SER 278 ATOM 7999 N SER 278 ATOM 8000 CA SER 278 ATOM 8001 CB SER 278 ATOM 8001 CB SER 278 ATOM 8002 OG SER 278 ATOM 8003 C SER 278 ATOM 8004 O SER 278 ATOM 8005 N VAL 279 ATOM 8006 CA VAL 279 ATOM 8007 CB VAL 279 ATOM 8008 CG1 VAL 279 ATOM 8009 CG2 VAL 279 ATOM 8010 C VAL 279 ATOM 8010 C VAL 279 ATOM 8011 O VAL 279 ATOM 8011 O VAL 279 ATOM 8012 N THR 280 ATOM 8013 CA THR 280 ATOM 8014 CB THR 280 ATOM 8015 OG1 THR 280 ATOM 8016 CG2 THR 280 ATOM 8017 C THR 280 ATOM 8016 CG2 THR 280 ATOM 8017 C THR 280 ATOM 8016 CG2 THR 280 ATOM 8017 C THR 280 ATOM 8016 CG2 THR 280 ATOM 8017 C THR 280 ATOM 8016 CG2 THR 280 ATOM 8017 C THR 280 ATOM 8018 O THR 280 ATOM 8019 N ASN 281 ATOM 8020 CA ASN 281 ATOM 8021 CB ASN 281 ATOM 8022 CG ASN 281 ATOM 8023 OD1 ASN 281 ATOM 8024 ND2 ASN 281 ATOM 8029 CB ALA 282 ATOM 8029 CB ALA 282 ATOM 8029 CB ALA 282 ATOM 8030 C ALA 282 ATOM 8030 C ALA 282 ATOM 8030 C ALA 282 ATOM 8031 O ALA 282 ATOM 8032 N THR 283 ATOM 8034 CB THR 283 ATOM 8035 OG1 THR 283	116. 076 80. 425 19. 664 1. 00 38. 58 116. 002 78. 958 20. 097 1. 00 36. 34 115. 319 78. 876 21. 445 1. 00 35. 16 115. 261 78. 134 19. 057 1. 00 32. 57 116. 914 82. 229 18. 140 1. 00 41. 99 117. 675 83. 002 18. 721 1. 00 44. 02 115. 916 84. 044 16. 863 1. 00 46. 53 116. 489 84. 277 15. 462 1. 00 48. 49 116. 268 85. 618 15. 044 1. 00 50. 90 114. 494 84. 586 16. 902 1. 00 46. 23 113. 529 83. 856 16. 701 1. 00 46. 82 114. 378 85. 884 17. 148 1. 00 46. 94 113. 081 86. 535 17. 202 1. 00 47. 82 113. 204 87. 899 17. 884 1. 00 48. 09 113. 419 86. 723 14. 808 1. 00 48. 26 111. 325 86. 829 15. 600 1. 00 48. 89 114. 189 87. 229 12. 514 1. 00 49. 95 113. 709 87	C C C C C O N C C O C O N C C O C O N C C C C

					FIC	G. 4-	165			(Continued)
ATOM ATOM ATOM ATOM	8036 8037 8038 8039	C 0 N	2 THR THR THR SER	283 283 283 284	114. 736 114. 074 115. 098 113. 123	73. 595 73. 403 73. 263 72. 482	11. 265 14. 125 14. 774 14. 073	1.00 37.32 1.00 33.58 1.00 34.31 1.00 32.05	B B B	C C O N
ATOM ATOM ATOM ATOM ATOM	8040 8041 8042 8043 8044	CA CB OG C	SER SER SER SER SER	284 284 284 284 284	113. 250 111. 935 111. 722 113. 638 113. 003	71. 230 70. 893 71. 761 70. 090 69. 865	14.800 15.507 16.605 13.883 12.850	1.00 30.43 1.00 28.61 1.00 29.31 1.00 30.34 1.00 31.22	B B B B	C C O C
ATOM ATOM ATOM ATOM ATOM	8045 8046 8047 8048 8049	N CA CB CG2	ILE ILE ILE ILE ILE	285 285 285 285 285	114. 684 115. 130 116. 660 117. 103 117. 383	69. 367 68. 241 68. 037 66. 979 69. 350	14. 260 13. 457 13. 546 12. 548 13. 250	1.00 29.19 1.00 28.80 1.00 29.35 1.00 29.12 1.00 30.38	B B B B	N C C C C
ATOM ATOM ATOM ATOM ATOM	8050 8051 8052 8053 8054		ILE ILE ILE GLN GLN	285 285 285 286 286	117. 408 114. 429 114. 472 113. 775 113. 067	70. 303 66. 996 66. 694 66. 278 65. 076	14. 428 13. 976 15. 168 13. 078 13. 457	1.00 34.47 1.00 28.14 1.00 30.23 1.00 25.84 1.00 24.81	B B B B	C C O N C
ATOM ATOM ATOM ATOM ATOM	8055 8056 8057 8058 8059	CB CG CD OE1	GLN GLN GLN GLN GLN	286 286 286 286 286	111. 852 111. 169 109. 928 109. 253 109. 614	64. 886 63. 547 63. 417 62. 388 64. 461	12. 550 12. 715 11. 868 11. 894 11. 110	1.00 23.81 1.00 23.29 1.00 23.98 1.00 25.22 1.00 23.87	B B B B	C C C O N
ATOM ATOM ATOM ATOM ATOM	8060 8061 8062 8063 8064	C O N CA CB	GLN GLN ILE ILE ILE	286 286 287 287 287	113. 955 114. 832 113. 723 114. 458 115. 193	63. 838 63. 732 62. 908 61. 655 61. 481	13. 386 12. 526 14. 307 14. 346 15. 694	1.00 25.74 1.00 26.39 1.00 24.54 1.00 23.40 1.00 21.87	B B B B	C O N C C
ATOM ATOM ATOM ATOM ATOM	8065 8066 8067 8068	CG2 CG1	ILE ILE ILE ILE ILE	287 287 287 287 287 287	115. 925 116. 180 117. 054 113. 394 112. 729	60. 143 62. 632 62. 506 60. 578 60. 204	15. 728 15. 887 17. 113 14. 186 15. 142	1.00 20.61 1.00 19.27 1.00 20.58 1.00 24.59	B B B B	C C C C
ATOM ATOM ATOM ATOM ATOM	8070 8071 8072 8073	N CA CB OG1	THR THR THR THR THR	288 288 288 288 288	113. 219 112. 205 111. 964 113. 172 111. 510	60. 093 59. 088 58. 927 58. 516 60. 255	12. 966 12. 708 11. 188 10. 539 10. 593	1.00 25.43 1.00 26.10 1.00 26.69 1.00 26.37 1.00 25.25	B B B B	N C C O
ATOM ATOM ATOM ATOM ATOM	8075 8076 8077 8078	C O N CA CB	THR THR ALA ALA ALA	288 288 289 289 289	112. 529 113. 687 111. 484 111. 638 110. 271	57. 741 57. 379 57. 011 55. 705 55. 151	13. 335 13. 503 13. 702 14. 325	1. 00 26. 85 1. 00 27. 04 1. 00 28. 37 1. 00 27. 90 1. 00 26. 91	B B B B	C C O N C
ATOM ATOM ATOM ATOM ATOM	8080 8081 8082 8083	C O N CD	ALA ALA PRO PRO PRO	289 289 290 290 290	112. 348 112. 550 112. 758 112. 903	55. 740 55. 038 53. 577 53. 280 52. 569	14. 710 13. 380 12. 205 13. 895 15. 328 13. 089	1.00 20.91 1.00 27.44 1.00 28.30 1.00 26.01 1.00 24.74 1.00 25.29	B B B B	C C O N C
	5551	J. I	1110	<i>450</i>	110. 710	U4. UUJ	10.003	1.00 40.43	D	С

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					FIC	G. 4-	166			(Continued)
ATOM	8085	СВ	PRO	290	113. 949	51.587	14. 138		В	С
ATOM	8086	CG	PRO	290	114. 151	52.467	15. 342	1.00 25.10	В	C
ATOM	8087	C	PRO	290	112. 465	51.931	12.110	1.00 25.85	В	C
ATOM	8088	0	PRO	290	111. 255	51.961	12. 330	1.00 25.95	В	0
ATOM	8089 8090	N CA	ALA	291	112. 988	51.345	11.038	1.00 25.39	В	N
ATOM ATOM	8091	CA CB	ALA ALA	291 291	112. 143	50.730	10.024	1.00 26.17	В	C
ATOM	8092	С	ALA	291 291	112. 987 111. 337	50. 271	8.846	1.00 26.28	В	C
ATOM	8093	Õ	ALA	291	110. 203	49. 568 49. 331	10. 573 10. 145	1.00 27.18 1.00 27.46	В	C
ATOM	8094	N	SER	292	111. 916	48. 843	11. 521	1.00 27.40	B B	O N
ATOM	8095	CA	SER	292	111. 220	47. 704	12. 103	1.00 27.34	В	C
ATOM	8096	CB	SER	292	112. 161	46. 892	12. 993	1.00 28.19	В	C
ATOM	8097	0G	SER	292	112. 525	47.626	14. 145	1.00 20.00	В	ő
ATOM	8098	Ċ	SER	292	110. 027	48. 182	12. 922	1.00 28.13	В	Č
ATOM	8099	0	SER	292	109.176	47.376	13. 307	1.00 29.52	В	ŏ
ATOM	8100	N	MET	293	109.976	49.487	13. 190	1.00 25.00	B	Ň
ATOM	8101	CA	MET	293	108.881	50.072	13.955	1.00 24.80	В	Č
ATOM	8102	CB	MET	293	109. 387	51.173	14.892	1.00 24.61	В	Č
ATOM	8103	CG	MET	293	110. 231	50.703	16.060	1.00 26.88	В	C
ATOM	8104	SD	MET	293	109. 323	49.647	17. 189	1.00 27.80	В	S C
ATOM	8105	CE	MET	293	110.457	48.319	17.438	1.00 25.74	В	
ATOM	8106	C	MET	293	107. 836	50.677	13.027	1.00 24.57	В	C
ATOM	8107	0	MET	293	106.641	50.528	13. 252	1.00 25.32	В	0
ATOM	8108	N	LEU	294	108. 292	51.360	11.983	1.00 24.37	В	N
ATOM ATOM	8109	CA	LEU	294	107. 393	52.008	11.041	1.00 23.80	В	C C C
ATOM	8110 8111	CB CG	LEU LEU	294 294	108. 183 108. 945	52.930	10.114	1.00 23.40	В	C
ATOM	8112		LEU	294 294	108. 945	54. 072 54. 787	10.786	1.00 24.87	В	C
ATOM	8113		LEU	294	103. 800	55.037	9. 758 11. 440	1.00 22.08	В	C
ATOM	8114	C	LEU	294	106.540	51.059	10. 204	1.00 23.08 1.00 23.95	B B	C C
ATOM	8115	ŏ	LEU	294	105. 714	51.510	9.422	1.00 25.36	В	0
ATOM	8116	N	ILE	295	106. 724	49. 754	10.357	1.00 23.92	В	N
ATOM	8117	CA	ILE	295	105. 923	48. 812	9.580	1.00 25.26	В	C
ATOM	8118	CB	ILE	295	106.601	47.444	9.453	1.00 26.06	B	Č
ATOM	8119	CG2	ILE	295	107. 972	47.595	8.812	1.00 26.54	В	č
ATOM	8120		ILE	295	106.698	46.796	10.831	1.00 24.44	B	č
ATOM	8121		ILE	295	107. 211	45.388	10.789	1.00 28.37	В	Ċ
ATOM	8122	C	ILE	295	104. 564	48. 575	10. 221	1.00 26.01	В	Ċ
ATOM	8123	0	ILE	295	103. 805	47. 712	9.775	1.00 28.75	В	0
ATOM	8124	N	GLY	296	104. 263	49. 328	11.273	1.00 24.77	В	N
ATOM	8125	CA	GLY	296	102. 992	49. 167	11.951	1.00 22.28	В	C
ATOM	8126	C	GLY	296	102.908	50.040	13.182	1.00 21.29	В	C
ATOM	8127	0	GLY	296	103.820	50. 818	13.447	1.00 20.80	В	0
ATOM	8128	N CA	ASP	297	101.818	49. 920	13.935	1.00 20.38	В	N
ATOM ATOM	8129 8130	CA CB	ASP	297	101.654	50. 718	15.141	1.00 20.14	В	C
ATOM	8131	CG	ASP ASP	297 207	100.366	50. 339	15.874	1.00 21.58	В	C
ATOM	8132	0D1		297 297	99. 109 98. 016	50. 665 50. 234	15.078	1.00 22.60 1.00 25.00	В	C
ATOM	8133	0D1		297	98.010	50. 254 51. 350	15.502 14.041	1.00 25.00	B B	0
111 (111	0100	UUU	1101	431	99. LUU	01.000	14.041	1.00 44.10	D	0

					FIC	١	167			(Continued)
ATOM ATOM	8134 8135		ASP		102. 845	50. 481	16.065	1.00 20.31	В	C
ATOM	8136		ASP HIS		103. 419 103. 220	49.390	16.096	1.00 20.82	В	0
ATOM	8137		HIS		103. 220	51.508 51.384	16. 814 17. 734	1.00 16.87 1.00 16.48	В	N
ATOM	8138		HIS		105.669	51.399	16. 968	1.00 10.48	B B	C C
ATOM	8139		HIS		105.868	52. 628	16. 137	1.00 14.31	В	C
ATOM	8140		2 HIS		106. 539	53. 775	16. 391	1.00 10.39	В	Č
ATOM	8141		HIS		105. 264	52. 802	14. 909	1.00 11.35	В	N
ATOM	8142		HIS		105.551	54.005	14. 445	1.00 11.25	B	Č
ATOM	8143		HIS		106.323	54.616	15.326	1.00 11.96	B	Ň
ATOM	8144	C	HIS		104. 274	52.560	18.693	1.00 15.84	В	C
ATOM	8145	0	HIS		103.484	53.476	18.505	1.00 17.04	В	0
ATOM	8146	N	TYR		105. 127	52. 539	19.706	1.00 15.50	В	N
ATOM ATOM	8147	CA	TYR		105.163	53. 599	20.698	1.00 15.35	В	C
ATOM	8148 8149	CB CG	TYR TYR		104.640	53.095	22. 047	1.00 14.51	В	C
ATOM	8150		TYR		103. 343 102. 120	52. 320	22.037	1.00 14.30	В	C
ATOM	8151		TYR		102. 120	52. 973 52. 269	21.942 22.019	1.00 13.49	В	C
ATOM	8152		TYR		100. 324	50. 933	22. 198	1.00 15.63 1.00 14.56	B B	C C
ATOM	8153		TYR		102. 150	50. 216	22. 273	1.00 14.50	В	C
ATOM	8154	CZ	TYR		100.943	50. 891	22. 186	1.00 15.73	В	Č
ATOM	8155	OH	TYR		99.756	50.197	22. 286	1.00 15.37	В	ŏ
ATOM	8156	C	TYR	299		54.084	20.952	1.00 16.54	B	č
ATOM	8157	0	TYR	299		53. 364	20.732	1.00 15.53	` B	0
ATOM	8158	N	LEU	300		55. 316	21. 428	1.00 16.67	В	N
ATOM ATOM	8159 8160	CA CB	LEU LEU	300		55. 853	21.818	1.00 17.75	В	C
ATOM	8161	CG	LEU	300 300		57. 367	21.654	1.00 18.54	В	C
ATOM	8162		LEU	300		58. 059 57. 535	22. 183 21. 429	1.00 20.06 1.00 20.50	В	C
ATOM	8163		LEU	300		59. 567	22. 024	1.00 20.50	B B	C C
ATOM	8164	Č	LEU	300		55. 477	23. 294	1.00 20.10	В	C
ATOM	8165	0	LEU	300		55. 783	23. 935	1.00 20.71	В	ŏ
ATOM	8166	N	CYS	301		54.805	23.849	1.00 18.50	B	Ň
ATOM	8167	CA	CYS	301		54.418	25. 252	1.00 20.22	B	Ċ
ATOM	8168	CB	CYS	301		52.907	25. 375	1.00 20.55	В	C
ATOM ATOM	8169	SG	CYS	301		51.905	24. 722	1.00 26.11	В	S
ATOM	8170 8171	C 0	CYS CYS	301		54. 842	26. 194	1.00 20.82	В	C
ATOM	8172	N	ASP	301 302		54. 579	27. 395	1.00 21.62	В	0
ATOM	8173	CA	ASP	302		55. 496 55. 968	25. 662 26. 481	1.00 22.13	В	N
ATOM	8174	CB	ASP	302		54. 810	27. 014	1.00 20.03 1.00 20.49	B B	C
ATOM	8175	CG	ASP	302		55. 296	27. 868	1.00 25.77	В	C C
ATOM	8176	0D1	ASP	302		55. 344	29. 109	1.00 26.02	В	0
ATOM	8177	0D2	ASP	302		55. 664	27. 297	1.00 27.73	В	0
ATOM	8178	C	ASP	302	112.959	56. 894	25.711	1.00 20.08	B	Č
ATOM	8179	0	ASP	302		56. 596	24. 586	1.00 19.30	В	Ö
ATOM	8180	N	VAL	303		58.010		1.00 20.41	В	N
ATOM ATOM	8181	CA	VAL	303		59.000		1.00 20.36	В	C
UIOI	8182	CB	VAL	303	113.435	60. 316	25. 470	1.00 19.97	В	C

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			-		FI	G. 4-	168			(Continued)
ATOM ATOM	8183 8184		VAL VAL	303 303	114.387	61.347	24.857	1.00 20.23	В	C
ATOM	8185	CGZ	VAL	303	112. 260 115. 267		24.540	1.00 17.52	В	C
ATOM	8186	0	VAL	303	113. 207		26. 788 27. 939	1.00 21.02	В	C
ATOM	8187	N	THR		114. 930		26.389	1.00 19.39	В	0 N
ATOM	8188	CA	THR		117. 639		27.332	1.00 21.38 1.00 21.48	B B	N
ATOM	8189	CB	THR		118.008		28.046	1.00 21.48	B	C C
ATOM	8190	0G1			116.869		28.751	1.00 19.77	В	0
ATOM	8191		THR		119.136		29. 026	1.00 19.55	В	C
ATOM	8192	Č	THR		118. 925	59. 851	26. 729	1.00 22.96	В	Č
ATOM	8193	Ŏ	THR	304	119.579	59. 159	25. 952	1.00 25.30	В	ŏ
ATOM	8194	N	TRP	305	119.307	61.069	27. 102	1.00 22.41	B	Ň
ATOM	8195	CA	TRP	305	120.545	61.643	26. 583	1.00 21.86	B	Ĉ ·
ATOM	8196	CB	TRP	305	120.696	63.114	26.975	1.00 20.21	B	č
ATOM	8197	CG	TRP	305	119.682	64.002	26.354	1.00 18.90	B	Č
ATOM	8198	CD2	TRP	305	119.834	64.751	25.150	1.00 18.79	B	Č
ATOM	8199		TRP	305	118.614	65.413	24.917	1.00 20.14	В	C C
ATOM	8200		TRP	305	120.885	64.928	24. 243	1.00 18.65	В	C
ATOM	8201		TRP	305	118. 414	64.232	26.794	1.00 17.49	В	C
ATOM	8202		TRP	305	117. 764	65.077	25.938	1.00 18.37	В	N
ATOM	8203		TRP	305	118.413	66.242	23.812	1.00 19.16	. В	C
ATOM	8204		TRP	305	120.689	65.746	23. 152	1.00 19.59	В	С
ATOM	8205		TRP	305	119.459	66. 395	22.943	1.00 21.43	В	C
ATOM	8206	C	TRP	305	121.722	60.875	27. 148	1.00 22.21	В	C
ATOM	8207	0	TRP	305	121.743	60. 552	28. 338	1.00 21.63	В	0
ATOM	8208	N	ALA	306	122.697	60. 591	26. 285	1.00 22.53	В	N
ATOM	8209	CA	ALA	306	123. 899	59.864	26.673	1.00 21.31	В	C
ATOM ATOM	8210 8211	CB C	ALA	306	124. 350	58.969	25. 533	1.00 20.65	В	C C C
ATOM	8212	0	ALA ALA	306 306	124.975	60.882	27.000	1.00 21.97	В	
ATOM	8213	N	THR	300 307	125.675 125.086	60.767	28.007	1.00 20.32	В	0
ATOM	8214	CA	THR	307	126.057	61. 885 62. 964	26. 133	1.00 23.85	В	N
ATOM	8215	CB	THR	307	127. 285	62.744	26. 284 25. 411	1.00 24.42 1.00 22.67	B B	C
ATOM	8216	OG1	THR	307	126. 894	62. 855	24. 040	1.00 25.33	В	C 0
ATOM	8217		THR	307	127. 892	61.374	25.659	1.00 20.33	В	C
ATOM	8218	C	THR	307	125. 397	64. 250	25. 812	1.00 25.73	В	C
ATOM	8219	Ō	THR	307	124. 177	64. 326	25. 731	1.00 28.17	В	Ö
ATOM	8220	N	GLN	308	126. 210	65. 249	25. 479	1.00 26.09	В	Ň
ATOM	8221	CA	GLN	308	125.699	66.540	25.022	1.00 24.49	В	Ċ
ATOM	8222	CB	GLN	308	126.762	67.634	25.175	1.00 22.95	B	Č
ATOM	8223	CG	GLN	308	127.301	67.811	26.574	1.00 21.20	B	Č
ATOM	8224	CD	GLN	308	126.256	68. 296	27.548	1.00 20.30	. B	Č
ATOM	8225		GLN	308	126.477	68. 290	28.754	1.00 23.08	В	0
ATOM	8226		GLN	308	125.116	68.727	27.032	1.00 21.02	В	N
ATOM	8227	C	GLN	308	125. 284	66.501	23.569	1.00 25.09	В	Ċ
ATOM	8228	0	GLN	308	124. 612	67.411	23. 095	1.00 26.23	В	0
ATOM	8229	N	GLU	309	125. 687	65. 459	22.855	1.00 25.59	В	N
ATOM	8230	CA	GLU	309	125. 370	65. 374	21.440	1.00 26.16	В	C
ATOM	8231	CB	GLU	309	126. 581	65.807	20.627	1.00 25.99	В	C

	FIG. 4-169	(Continued)
ATOM 8259 CB SER ATOM 8260 OG SER ATOM 8261 C SER ATOM 8262 O SER ATOM 8263 N LEU ATOM 8264 CA LEU ATOM 8265 CB LEU ATOM 8266 CG LEU ATOM 8266 CG LEU ATOM 8268 CD2 LEU ATOM 8269 C LEU ATOM 8270 O LEU ATOM 8271 N GLN ATOM 8271 N GLN ATOM 8272 CA GLN ATOM 8273 CB GLN ATOM 8274 CG GLN ATOM 8274 CG GLN ATOM 8275 CD GLN ATOM 8276 OE1 GLN ATOM 8277 NE2 GLN	309	Continued B C B C C B C C B C C B C C C C C C C
	14 111. 412 54. 045 22. 513 1. 00 22. 96 15 111. 984 52. 372 21. 108 1. 00 22. 35	B O B N

										(Continued)
				-	F I (G. 4 -	170			•
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8281 8282 8283 8284 8285 8286 8287 8288	CE2 CE3 CD1	TRP TRP TRP TRP TRP TRP TRP TRP	315 315 315 315 315 315	110. 672 110. 769 111. 376 110. 678 111. 654 109. 325 112. 705	52. 262 52. 440 53. 741 54. 940 55. 901 55. 295 54. 018	20. 484 18. 968 18. 540 18. 176 17. 824 18. 113 18. 405	1. 00 21. 75 1. 00 21. 09 1. 00 21. 09 1. 00 19. 81 1. 00 20. 24 1. 00 17. 16 1. 00 21. 12	B B B B B	C C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8289 8290 8291 8292 8293 8294 8295	CZ2 CZ3	TRP TRP TRP TRP TRP LEU LEU	315 315 315 315 315 315 316 316	112. 880 111. 321 108. 992 109. 990 110. 118 110. 877 108. 799 108. 159	55. 310 57. 197 56. 588 57. 522 50. 880 49. 922 50. 772 49. 502	17. 974 17. 413 17. 704 17. 359 20. 790 20. 941 20. 872 21. 184	1.00 21.84 1.00 18.97 1.00 20.13 1.00 19.26 1.00 22.37 1.00 24.80 1.00 21.02 1.00 20.90	B B B B B	N C C C C O N
ATOM ATOM ATOM ATOM ATOM ATOM	8296 8297 8298 8299 8300 8301	CB CG CD1 CD2 C	LEU LEU LEU LEU LEU	316 316 316 316 316 316	107. 653 106. 866 107. 786 106. 223 106. 995 106. 161	49. 544 48. 358 47. 157 48. 783 49. 228 50. 098	22. 628 23. 194 23. 408 24. 501 20. 229 20. 000	1.00 19.84 1.00 19.46 1.00 18.22 1.00 16.50 1.00 20.90 1.00 22.41	B B B B B	C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8302 8303 8304 8305 8306 8307 8308	N CA CB CG CD NE CZ	ARG ARG ARG ARG ARG ARG	317 317 317 317 317 317 317	106. 941 105. 851 106. 154 107. 248 107. 524 108. 347 108. 925	48. 026 47. 678 46. 362 46. 480 45. 149 45. 314 44. 313	19. 666 18. 753 18. 035 16. 993 16. 321 15. 128 14. 476	1.00 19.89 1.00 20.30 1.00 20.73 1.00 23.49 1.00 24.95 1.00 25.57 1.00 26.73	B B B B B	N C C C C N C
ATOM ATOM ATOM ATOM ATOM ATOM	8309 8310 8311 8312 8313 8314 8315	NH2 C O N CA	ARG ARG ARG ARG ARG	317 317 317 317 318 318	108. 775 109. 656 104. 537 104. 541 103. 415 102. 117	43. 061 44. 567 47. 545 47. 266 47. 747 47. 621	14. 897 13. 401 19. 512 20. 713 18. 820 19. 476	1.00 23.81 1.00 29.12 1.00 19.31 1.00 17.59 1.00 18.54 1.00 17.04	B B B B	N N C O N C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8316 8317 8318 8319 8320 8321		ARG ARG ARG ARG ARG ARG ARG	318 318 318 318 318 318 318	100. 970 99. 608 98. 613 97. 326 96. 320 96. 464 95. 180	47. 781 47. 794 48. 660 48. 672 49. 478 50. 342 49. 428	18. 483 19. 164 18. 414 19. 092 18. 771 17. 771 19. 460	1. 00 17. 09 1. 00 17. 74 1. 00 16. 48 1. 00 16. 05 1. 00 17. 02 1. 00 13. 59 1. 00 12. 42	B B B B B	C C C N C N
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8322 8323 8324 8325 8326 8327 8328 8329	C O N CA CB CG2 CG1	ARG ARG ILE ILE ILE ILE	318 319 319 319 319 319 319	102. 085 101. 569 102. 627 102. 757 103. 006 103. 268 101. 793 100. 524	46. 251 46. 103 45. 251 43. 912 42. 848 41. 519 42. 732 42. 425	20. 132 21. 234 19. 440 20. 007 18. 949 19. 621 18. 036 18. 781	1. 00 15. 28 1. 00 15. 74 1. 00 15. 27 1. 00 15. 37 1. 00 15. 60 1. 00 17. 64 1. 00 15. 37 1. 00 15. 37	B B B B B B	C O N C C C C

					DI	0 4	1 77 1			(Continued)
					P 1.0	٠ 4	- 171	•		
ATOM	8330		ILE		104.036	44. 122			В	C
ATOM	8331	0	ILE		105.145	44. 086			В	0
ATOM	8332	N	GLN		103.850				В	N
ATOM ATOM	8333 8334	CA CB	GLN GLN		104. 923				В	C
ATOM	8335	CG	GLN	320 320	104. 293	45. 341			В	C
ATOM	8336	CD	GLN	320	103. 383 102. 833	46. 495 47. 250			В	C
ATOM	8337	0E		320	102. 555	47. 509		1.00 17.00	B B	C 0
ATOM	8338		2 GLN	320	101.566	47. 633		1.00 16.02	В	N N
ATOM	8339	C	GLN	320	105.964	43.663		1.00 10.40	В	C
ATOM	8340	0	GLN	320	106.399	43.654		1.00 20.18	В	ŏ
ATOM	8341	N	ASN	321	106.382	42.800		1.00 19.64	B	N
ATOM	8342	CA	ASN	321	107.420	41.846		1.00 21.44	B	Ċ
ATOM	8343	CB	ASN	321	106.950	40.399	22.719	1.00 23.79	В	С
ATOM	8344	CG	ASN	321	106.409	40.085	21. 332	1.00 27.68	В	С
ATOM	8345		ASN	321	106. 593	40.839	20.374	1.00 28.16	В	0
ATOM	8346		2 ASN	321	105.745	38. 934	21. 255	1.00 30.91	В	N
ATOM ATOM	8347 8348	C	ASN	321	108.658	42.087	22.036	1.00 21.63	B .	C
ATOM	8349	O N	ASN TYR	321 322	109.533	41. 228	21.940	1.00 23.87	В	0 ·
ATOM	8350	CA	TYR	322	108. 735 109. 873	43. 275	21.444	1.00 20.56	В	N
ATOM	8351	CB	TYR	322	109.605	43. 644 43. 208	20. 613 19. 178	1.00 18.63 1.00 18.95	В	C
ATOM	8352	CG	TYR	322	110.766	43. 362	18. 228	1.00 18.95	B B	C C
ATOM	8353	CD1		322	111.086	44. 604	17. 677	1.00 21.18	В	C
ATOM	8354		TYR	322	112.118	44. 733	16. 759	1.00 22.17	В	Č
ATOM	8355		TYR	322	111.520	42. 252	17. 840	1.00 20.55	В	Č
ATOM	8356		TYR	322 ,	112.557	42.372	16.925	1.00 21.33	B	č
ATOM	8357	CZ	TYR	322	112.847	43.611	16.387	1.00 22.88	B	Č
ATOM	8358	OH	TYR	322	113.855	43.726	15.461	1.00 28.00	В	Ô
ATOM	8359	C	TYR	322	110.115	45.149	20.678	1.00 18.95	В	С
ATOM	8360	0	TYR	322	109. 240	45. 945	20. 338	1.00 20.45	В	0
ATOM ATOM	8361	N	SER	323	111. 299	45. 537	21.139	1.00 18.50	В	N
ATOM	8362 8363	CA CB	SER SER	323	111.657	46.946	21. 233	1.00 17.89	В	<u>C</u>
ATOM	8364	OG	SER	323 323	111.623	47.418	22. 684	1.00 18.88	В	C
ATOM	8365	C	SER	$\begin{array}{c} 323 \\ 323 \end{array}$	112.602 113.057	46. 740 47. 131	23. 444	1.00 21.21	В	0
ATOM	8366	Ö	SER	323	113. 851	46. 190	20. 677 20. 657	1.00 16.99 1.00 15.79	В	C
ATOM	8367	N	VAL	324	113. 360	48. 345	20. 230	1.00 15.79	B B	0 N
ATOM	8368	CA	VAL	324	114.672	48. 638	19.664	1.00 10.31	В	N C
ATOM	8369	CB	VAL	324	114.612	48. 684	18. 126	1.00 17.33	· В	C
ATOM	8370	CG1	VAL	324	113. 454	49.550	17. 692	1.00 22.04	B	Č
ATOM	8371	CG2	VAL	324	. 115.901	49. 257	17.565	1.00 20.08	B	č
ATOM	8372	C	VAL	324	115. 201	49.970	20. 151	1.00 16.54	\tilde{B}	č
ATOM	8373	0	VAL	324	114. 460	50.946	,20. 243	1.00 19.05	В	0
ATOM	8374	N	MET	325	116. 487	50.011	20. 463	1.00 15.89	В	N
ATOM	8375	CA	MET	325	117. 104	51. 243	20. 914	1.00 16.61	В	С
ATOM	8376	CB	MET	325	118.053	50. 997	22. 083	1.00 17.97	В	С
ATOM ATOM	8377	CG	MET	325	118. 682	52. 280	22. 597	1.00 19.56	В	Ċ
VION	8378	SD	MET	325	119. 851	52.014	23. 915	1.00 22.61	В	S
				S	UBSTITUTE	SHEET ((RULE 26	5)		

				* A					•	(Cambinana)
					FI	G. 4 -	172			(Continued)
ATOM	8379	CE	MET	325	118. 765		25. 211	1.00 21.39	В	C
ATOM	8380	C	MET	325	117. 895		19. 782	1.00 17.82	В	C
ATOM	8381	0	MET	325	118.658		19.082	1.00 15.28	В	0
ATOM	8382	N	ASP	326	117. 698		19.607	1.00 18.85	В	N
ATOM	8383	CA	ASP	$\frac{326}{226}$	118. 409		18. 591	1.00 21.89	В	C
ATOM	8384	CB	ASP	326	117. 436		17. 695	1.00 22.04	В	C
ATOM ATOM	8385 8386	CG	ASP ASP	$\begin{array}{c} 326 \\ 326 \end{array}$	117.533		16. 244	1.00 23.15	В	C
ATOM	8387		ASP	326	116.800 118.334		15. 418 15. 922	1.00 25.35 1.00 23.67	В	0
ATOM	8388	C	ASP	326	119. 299		19. 327	1.00 23.07	B B	0
ATOM	8389	ŏ	ASP	326	118. 896		20. 335	1.00 24.54	В	C 0
ATOM	8390	N	ILE	327	120. 521	55.062	18.842	1.00 25.03	В	N N
ATOM	8391	.CA	ILE	327	121. 451	55. 986	19.459	1.00 27.44	В	C
ATOM	8392	CB	ILE	327	122. 713	55. 263	19. 936	1.00 27.10	В	č
ATOM	8393		ILE	327	123. 697		20. 515	1.00 27.85	В	č
ATOM	8394		ILE	327	122. 321	54. 221	20. 984	1.00 25.49	B	č
ATOM	8395	CD1		327	123.476	53. 506	21.594	1.00 27.60	B	č
ATOM	8396	С	ILE	327	121.784	57.005	18. 395	1.00 29.15	B	č
ATOM	8397	0	ILE	327	122. 357	56.673	17.357	1.00 31.19	B	Ö
ATOM	8398	N	CYS	328	121.414	58. 250	18.653	1.00 30.14	В	N
ATOM	8399	CA	CYS	328	121.624	59. 298	17.684	1.00 31.56	В	С
ATOM	8400	C	CYS	328	122.624	60.356	18.084	1.00 32.64	В	C
ATOM	8401	0	CYS	328	122. 525	60.972	19. 153	1.00 33.03	В	0
ATOM	8402	CB	CYS	328	120. 286	59. 938	17. 366	1.00 32.73	В	C
ATOM	8403	SG	CYS	328	118. 979	58.689	17. 154	1.00 36.31	В	S
ATOM	8404	N	ASP	329	123. 596	60. 555	17. 200	1.00 32.72	В	N
ATOM	8405	CA	ASP	329	124. 639	61.542	17.406	1.00 32.74	В	C
ATOM	8406	CB	ASP	329	125. 997	60.975	16. 981	1.00 34.70	В	C
ATOM	8407	CG	ASP	329	126. 480	59.858	17.894	1.00 36.73	В	C
ATOM ATOM	8408 8409		ASP ASP	329	127.643	59. 431	17. 735	1.00 38.23	В	0
ATOM	8410	C	ASP	329	125. 706	59. 405	18.767	1.00 36.00	В	0
ATOM	8411	0	ASP	329 329	124. 320 123. 767	62. 781 62. 692	16.588	1.00 31.70	В	C
ATOM	8412	N	TYR	330	123. 101	63. 940	15. 494 17. 129	1.00 30.70	В	0
ATOM	8413	CA	TYR	330	124. 002	65. 191	16. 428	1.00 31.69 1.00 33.40	В	N
ATOM	8414	CB	TYR	330	124. 376	66. 354	17. 411	1.00 33.40	B B	C C
ATOM	8415	CG	TYR	330	124. 322	67.693	16. 728	1.00 30.81	В	C
ATOM	8416	CD1	TYR	330	123. 185	68.089	16. 030	1.00 29.73	В	C
ATOM	8417	CE1	TYR	330	123. 121	69. 326	15. 399	1.00 30.94	В	Č
ATOM	8418	CD2		330	125. 407	68.568	16. 777	1.00 30.62	В	Č
ATOM	8419	CE2		330	125. 356	69.814	16. 150	1.00 30.16	B	č
ATOM	8420	CZ	TYR	330	124. 206	70.186	15. 465	1.00 31.10	B	č
ATOM	8421	0H	TYR	330	124. 122	71.422	14. 867	1.00 29.92	В	ŏ
ATOM	8422	C	TYR	330	125.523	65.462	15.412	1.00 35.09	B	č
ATOM	8423	0	TYR	330	126.692	65.552	15.772	1.00 36.29	B	Ö
ATOM	8424	N	ASP	331	125. 149	65.600	14.146	1.00 37.07	В	N
ATOM	8425	CA	ASP	331	126. 123	65.886	13.106	1.00 39.50	В	C
ATOM	8426	CB	ASP	331	125.611	65. 391	11.756	1.00 39.77	В	C
ATOM	8427	CG	ASP	331	126.665	65. 464	10.677	1.00 40.31	В	С

			FIG. 4-173	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8429 OD2 ASI 8430 C ASI 8431 O ASI 8432 N GLI 8433 CA GLI 8434 CB GLI 8435 CG GLI 8436 CD GLI 8438 OE2 GLI 8439 C GLI 8440 O GLI 8441 N SER 8442 CA SER 8442 CA SER 8443 CB SER 8445 C SER 8446 O SER 8447 N SER 8448 CA SER 8449 CB SER 8447 N SER 8448 CA GLY 8451 C SER 8450 OG SER 8451 C SER 8451 C SER 8452 O SER 8453 N GLY 8455 C GLY 8456 O GLY 8457 N ARG 8458 CA ARG 8459 CB ARG 8457 N ARG 8458 CA ARG 8459 CB ARG 8459 CB ARG 8450 CG ARG 8461 CD ARG 8463 CZ ARG 8464 NH1 ARG 8465 NH2 ARG 8466 C ARG 8467 O ARG 8468 N TRP 8469 CA TRP	331 331 332 332 332 332 332 332 332 333 333	126. 387 65. 018 9. 543 1. 00 41. 37 B 127. 770 65. 966 10. 967 1. 00 40. 07 B 126. 355 67. 395 13. 062 1. 00 41. 15 B 125. 641 68. 126 12. 380 1. 00 44. 16 B 127. 358 67. 852 13. 802 1. 00 44. 16 B 127. 690 69. 271 13. 879 1. 00 47. 17 B 129. 367 70. 901 14. 922 1. 00 51. 70 B 130. 451 71. 028 15. 979 1. 00 54. 56 B 130. 203 70. 623 17. 136 1. 00 55. 51 B 131. 552 71. 528 15. 658 1. 00 56. 11 B 127. 791 69. 941 12. 517 1. 00 47. 83 B 128. 179 69. 175 11. 505 1. 00 44. 69 B 128. 312 69. 715 10. 161 1. 00 49. 93 B 129. 246 68. 835 9. 327 1. 00 50. 95 B 130. 521<	
ATOM ATOM ATOM	8469 CA TRP 8470 CB TRP 8471 CG TRP	337 337 337	100 055 00 010	N C C C
ATOM ATOM ATOM ATOM	8472 CD2 TRP 8473 CE2 TRP 8474 CE3 TRP 8475 CD1 TRP	337 337 337 337	120.670 65.059 17.214 1.00 17.75 B 120.550 66.390 17.671 1.00 17.16 B 121.374 64.137 17.997 1.00 15.36 B	C . C .
ATOM	8476 NEI TRP	337	119. 498 66. 224 15. 709 1. 00 19. 73 B 119. 827 67. 079 16. 736 1. 00 18. 61 B	C N

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					FIC	G. 4	174			(Continued)
ATOM	8477		2 TRP		121.110		18. 875	1.00 18.08	В	С
ATOM	8478	CZS			121.932			1.00 15.24	B	Ċ
ATOM	8479	CH:			121.798		19.622	1.00 16.71	В	Č
ATOM	8480	C	TRP		120.940		13. 188	1.00 31.57	В	C
ATOM	8481	0	TRP		119. 983		12.482	1.00 33.23	В	0
ATOM	8482	N	ASN		122.003			1.00 32.12	В	N
ATOM	8483	CA	ASN		122. 079		12.691	1.00 33.02	В	C
ATOM	8484	CB	ASN		123. 240		11.698	1.00 34.88	В	C
ATOM ATOM	8485 8486	CG	ASN ASN		122. 957		10.471	1.00 38.68	В	C
ATOM	8487		ASN R ASN		123. 595	62. 306	10. 251	1.00 39.82	В	0
ATOM	8488	C	ASN		121.984 122.216	60. 845 59. 294	9. 669 13. 693	1.00 38.06	В	N
ATOM	8489	Õ	ASN		123. 009	59. 364	14. 631	1.00 33.48 1.00 33.12	B B	C
ATOM	8490	Ň	CYS		121.419	58. 251	13. 499	1.00 33.12	В	O N
ATOM	8491	CA	CYS		121. 459	57. 104	14. 385	1.00 33.00	В	C .
ATOM .	8492	C	CYS		121. 924		13. 564	1.00 33.56	В	C
ATOM	8493	0	CYS		121.135	55. 296	12. 848	1.00 34.05	В	ŏ
ATOM	8494	CB	CYS		120.071	56.829	14.961	1.00 34.96	B	č
ATOM	8495	SG	CYS	339	118.997	58. 291	15.160	1.00 37.83	B	Š
ATOM	8496	N	LEU		123. 211	55.604	13.665	1.00 32.80	B	N
ATOM	8497	CA	LEU		123. 798	54.491	12.933	1.00 33.83	В	C
ATOM	8498	CB	LEU		125. 303	54. 413	13. 218	1.00 34.61	В	C
ATOM	8499	CG	LEU	340	126. 163	55. 530	12.609	1.00 34.61	В	C
ATOM ATOM	8500		LEU	340	127. 500	55. 633		1.00 31.70	В	C
ATOM	8501 8502	CDZ	LEU LEU	340	126. 352	55. 257	11.132	1.00 33.80	В	C
ATOM	8503	0	LEU	$\begin{array}{c} 340 \\ 340 \end{array}$	123. 152 123. 061	53. 151	13. 259	1.00 34.95	В	C
ATOM	8504	N	VAL	341	123. 001	52. 752 52. 457	14.418 12.220	1.00 34.65	В	0
ATOM	8505	CA	VAL	341	122. 003	51.152	12. 220	1.00 35.87 1.00 36.37	В	N
ATOM	8506	CB	VAL	341	121.981	50. 423	11.047	1.00 36.37	B B	C C
ATOM	8507		VAL	341	121.012	49. 256	11.175	1.00 37.20	В	C
ATOM	8508		VAL	341	121.532	51.391	9. 968	1.00 38.15	B	Č
ATOM	8509	C	VAL	341	122.957	50.305	13. 314	1.00 36.74	В	č
ATOM	8510	0	VAL	341	122.511	49.872	14.366	1.00 39.77	B	ŏ
ATOM		N	ALA	342	124. 200	50.073	12.913	1.00 35.94	В	N
ATOM	8512	CA	ALA	342	125. 134	49. 283	13.704	1.00 34.75	В	С
ATOM	8513	CB	ALA	342	126. 546	49.482	13. 178	1.00 34.41	В	C
ATOM	8514	C	ALA	342	125.095	49.609	15. 194	1.00 34.74	В	C
ATOM ATOM	8515 8516	0 N	ALA	342	125. 698	48. 897	16.001	1.00 36.76	В	0
ATOM	8516 8517	N CA	ARG ARG	343 343	124. 411	50.688	15.561	1.00 32.52	В	N
ATOM	8518	CB	ARG	343 343	124. 303	51.074	16.961	1.00 30.81	В	C
ATOM	8519	CG	ARG	343 343	124. 611 126. 063	52. 562 52. 922	17.120 16.844	1.00 32.62	В	C
ATOM	8520	CD	ARG	343	126. 345	54. 396	17. 131	1. 00 34. 14 1. 00 33. 56	B B	C
ATOM	8521	NE	ARG	343	127. 775	54. 692	17. 108	1.00 33.30	В	C N
ATOM	8522	CZ	ARG	343	128. 301	55. 885	17. 374	1.00 34.14	В	C
ATOM	8523		ARG	343	127. 516	56.907	17.680	1.00 33.88	В	N
ATOM	8524		ARG	343	129.615	56.052	17. 352	1.00 33.78	B	N
ATOM	8525	C	ARG	343	122. 919	50.751	17.535	1.00 29.28	B	Ċ

					FIG. 4-175	(Continued)
ATOM ATOM ATOM ATOM ATOM	8526 8527 8528 8529 8530 8531	O N CA CB CG CD	ARG GLN GLN GLN GLN GLN	343 344 344 344 344	122. 586 51. 143 18. 650 1. 00 28. 30 B 122. 121 50. 026 16. 763 1. 00 28. 05 B 120. 786 49. 625 17. 183 1. 00 28. 26 B 119. 944 49. 238 15. 974 1. 00 26. 68 B 118. 980 50. 296 15. 516 1. 00 30. 39 B 118. 091 49. 802 14. 399 1. 00 31. 50 B	N C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8532 8533 8534 8535 8536 8537 8538 8539		GLN GLN GLN HIS HIS HIS	344 344 344 345 345 345 345	117. 567 48. 685 14. 457 1. 00 31. 52 B 117. 905 50. 632 13. 378 1. 00 32. 84 B 120. 853 48. 431 18. 121 1. 00 28. 55 B 121. 655 47. 515 17. 919 1. 00 28. 32 B 120. 008 48. 436 19. 145 1. 00 28. 34 B 119. 977 47. 329 20. 085 1. 00 28. 01 B 120. 514 47. 753 21. 452 1. 00 28. 88 B 121. 973 48. 079 21. 443 1. 00 27. 88 B	O N C O N C C
ATOM ATOM ATOM ATOM ATOM ATOM	8540 8541 8542 8543 8544 8545 8546	CD2 ND1 CE1 NE2 C O N	HIS HIS HIS HIS HIS HIS	345 345 345 345 345 345 346	123.062 47.279 21.516 1.00 26.67 B 122.449 49.361 21.270 1.00 28.37 B 123.769 49.337 21.234 1.00 28.14 B 124.166 48.086 21.381 1.00 28.63 B 118.568 46.799 20.215 1.00 27.76 B 117.659 47.508 20.625 1.00 30.01 B 118.396 45.538 19.849 1.00 26.83 B	C N C N C O N
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8547 8548 8549 8550 8551 8552 8553 8554	CG1	ILE ILE ILE ILE ILE ILE ILE ILE	346 346 346 346 346 346 347	117. 102 44. 897 19. 899 1. 00 25. 72 B 116. 977 43. 842 18. 791 1. 00 25. 56 B 115. 655 43. 114 18. 919 1. 00 26. 17 B 117. 102 44. 517 17. 422 1. 00 26. 62 B 117. 180 43. 544 16. 263 1. 00 26. 42 B 116. 854 44. 218 21. 228 1. 00 26. 11 B 117. 736 43. 558 21. 776 1. 00 25. 75 B 115. 645 44. 396 21. 746 1. 00 26. 23 B	C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8555 8556 8557 8558 8559 8560 8561	CA CB CG CD OE1 OE2 C	GLU GLU GLU GLU GLU GLU GLU	347 347 347 347 347 347 347	115. 645 44. 396 21. 746 1. 00 26. 23 B 115. 260 43. 767 22. 994 1. 00 25. 82 B 115. 226 44. 777 24. 134 1. 00 25. 51 B 115. 282 44. 118 25. 505 1. 00 28. 20 B 115. 107 45. 094 26. 652 1. 00 29. 16 B 115. 667 46. 208 26. 592 1. 00 29. 18 B 114. 415 44. 736 27. 628 1. 00 32. 76 B 113. 873 43. 172 22. 799 1. 00 26. 44 B	N C C C C O O C
ATOM ATOM ATOM ATOM ATOM ATOM	8562 8563 8564 8565 8566 8567 8568	O N CA CB CG SD CE	GLU MET MET MET MET MET MET	347 348 348 348 348 348 348	112. 919 43. 889 22. 495 1. 00 26. 00 B 113. 770 41. 858 22. 957 1. 00 26. 58 B 112. 492 41. 181 22. 807 1. 00 27. 90 B 112. 270 40. 767 21. 345 1. 00 30. 41 B 113. 466 40. 132 20. 660 1. 00 34. 65 B 113. 695 38. 420 21. 117 1. 00 42. 21 B 112. 733 37. 597 19. 804 1. 00 38. 96 B	O N C C C S C
ATOM ATOM ATOM ATOM ATOM ATOM	8569 8570 8571 8572 8573 8574	C O N CA CB OG	MET MET SER SER SER SER	348 348 349 349 349 349	112. 371 39. 980 23. 732 1. 00 26. 60 B 113. 363 39. 472 24. 247 1. 00 26. 08 B 111. 135 39. 549 23. 950 1. 00 23. 99 B 110. 843 38. 423 24. 812 1. 00 21. 78 B 109. 989 38. 894 25. 997 1. 00 20. 79 B 109. 402 37. 809 26. 700 1. 00 21. 42 B	C O N C C O

					FΙ	G. 4	-176	,		(Continued))
ATOM	8575	С	SER	349	110. 084				מ	C	
ATOM	8576	ŏ	SER		109. 274				B B	C	
ATOM	8577	Ň	THR		110. 351				В	O N	
ATOM	8578	CA	THR		109.654				В	C	
ATOM	8579	CB	THR		110.603				В	Č	
ATOM	8580	0G1			111. 310			1.00 25.37	В	ŏ ·	
ATOM	8581	CG2	? THR		111.583	34. 299			В	Č	
ATOM	8582	C	THR		108. 561	34. 453			В	č	
ATOM	8583	0	THR		107. 732				В	ŏ	
ATOM	8584	N	THR		108.564	34.871	25.737		B	N	
ATOM	8585	CA	THR		107.601	34.366			B	Ĉ	
ATOM	8586	CB	THR		108. 332			1.00 23.36	В	C	
ATOM	8587	0G1			108. 989			1.00 25.67	В	0	
ATOM	8588	CG2		351	109. 378		27. 493	1.00 22.26	В	C	
ATOM	8589	C	THR	351	106.575		27. 171	1.00 21.07	В	С	
ATOM	8590	0	THR	351	105. 562		27.760	1.00 20.87	В	0	
ATOM	8591	N	GLY	352	106.839		26. 918	1.00 19.83	В	N	
ATOM	8592	CA	GLY	352	105.894		27. 325	1.00 19.36	В	C	
ATOM ATOM	8593	C	GLY	352	106. 182		26.672	1.00 18.63	В	C	
ATOM	8594 8595	O N	GLY TRP	352	106.633		25.531	1.00 20.78	В	0	
ATOM	8596	CA	TRP	353 353	105. 913 106. 156		27. 397	1.00 17.51	В	N	
ATOM	8597	CB	TRP	353 353	105. 195		26.907	1.00 15.30	В	C	
ATOM	8598	CG	TRP	353	105. 195		27. 587 29. 084	1.00 13.08	В	C	
ATOM	8599		TRP	353	104. 479		29. 877	1.00 9.17 1.00 7.79	В	C	
ATOM	8600		TRP	353	104. 739		31. 233	1.00 1.19	B B	C	
ATOM	8601		TRP	353	103. 671	40. 288	29. 574	1.00 10.72	В	C C	
ATOM	8602		TRP	353	105. 798	43. 195	29. 966	1.00 10.72	В	C	
ATOM	8603		TRP	353	105. 546	42. 791	31.265	1.00 10.10	В	N	
ATOM	8604		TRP	353	104. 217	40. 921	32. 281	1.00 10.66	В	C	
ATOM	8605		TRP	353	103.149	39. 524	30.625	1.00 10.40	В	Č	
ATOM	8606		TRP	353	103. 426	39.848	31.958	1.00 9.81	В	Č	
ATOM	8607	C	TRP	353	107. 594	41.796	27. 264	1.00 15.80	B	č	
ATOM	8608	0	TRP	353	108. 247	40.999	27. 931	1.00 16.59	B	Ŏ	
ATOM	8609	N	VAL	354	108. 092	42.946	26.819	1.00 13.84	В	N	
ATOM	8610	CA	VAL	354	109. 464	43. 338	27. 140	1.00 13.65	В	C	
ATOM	8611	CB	VAL	354	110. 135	44.096	25.960	1.00 16.06	В	С	
ATOM	8612		VAL	354	111.506	44.646	26.400	1.00 12.56	В	C	
ATOM	8613		VAL	354	110. 284	43. 163	24. 751	1.00 12.49	В	C	
ATOM	8614	C	VAL	354	109. 486	44. 248	28. 368	1.00 13.83	В	C	
ATOM ATOM	8615 8616	O N	VAL	354	108. 716	45. 197	28. 456	1.00 13.93	В	0	
ATOM	8617	CA	GLY GLY	355 355	110.373	43.957	29. 313	1.00 14.87	В	Ŋ	
ATOM	8618	C	GLY	355	110. 467	44. 769	30. 519	1.00 16.09	В	C	
ATOM	8619	Õ	GLY	355	109.333	44. 554	31.513	1.00 16.34	В	C	
ATOM	8620	N	ARG	356	108. 347 109. 456	43.877	31. 206	1.00 18.25	В	0	
ATOM	8621	CA	ARG	356	109. 400	45. 126 44. 953	32. 706	1.00 15.16	В	N	
ATOM	8622		ARG	356	108. 404	44. <i>9</i> 03 45. 494	33. 701 35. 066	1.00 16.32 1.00 14.18	B	C	
ATOM	8623		ARG	356	110.001	44. 668		1.00 14.18	B B	C C	
				555	110.001	* ** 000	00.001	1.00 10.44	Ŋ	U	

				(Continued)
			FIG. 4-177	, a a a a a a a a a a a a a a a a a a a
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8624 CD ARC 8625 NE ARC 8626 CZ ARC 8627 NH1 ARC 8628 NH2 ARC 8629 C ARC 8630 O ARC 8631 N PHE 8632 CA PHE 8633 CB PHE 8634 CG PHE 8635 CD1 PHE 8636 CD2 PHE 8636 CD2 PHE 8637 CE1 PHE 8638 CE2 PHE 8639 CZ PHE 8639 CZ PHE 8640 C PHE 8640 C PHE 8641 O PHE 8641 O PHE 8642 N ARG 8644 CB ARG 8644 CB ARG	356 356 356 356 356 357 357 357 357 357 357	FIG. 4 - 177 110. 169	C C C C C C C C C C C C C C C C C C C
ATOM	8645 CG ARG		108. 451 51. 346 30. 559 1. 00 19. 99 B	C
ATOM	8646 CD ARG		108. 074 52. 820 30. 338 1. 00 22. 48 B	C
ATOM	8647 NE ARG		108. 633 53. 708 31. 362 1. 00 24. 20 B	N
ATOM	8648 CZ ARG	358	109. 204 54. 890 31. 117 1. 00 24. 69 B	C
ATOM	8649 NH1 ARG	358	109. 304 55. 358 29. 875 1. 00 21. 14 B	N
ATOM	8650 NH2 ARG	358	109. 696 55. 603 32. 121 1. 00 24. 33 B	N
ATOM	8651 C ARG	358	109. 707 48. 784 29. 646 1. 00 20. 57 B	C
ATOM	8652 O ARG	358	110. 302 48. 704 30. 722 1. 00 22. 16 B	O
ATOM	8653 N PRO	359	110. 355 48. 723 28. 473 1. 00 20. 23 B	N
ATOM	8654 CD PRO	359	109. 783 48. 894 27. 124 1. 00 20. 61 B	C
ATOM	8655 CA PRO	359	111. 816 48. 564 28. 411 1. 00 20. 48 B	C
ATOM	8656 CB PRO	359	112. 137 48. 916 26. 959 1. 00 19. 85 B	C
ATOM	8657 CG PRO	359	110. 919 48. 431 26. 229 1. 00 21. 21 B	C
ATOM	8658 C PRO	359	112. 527 49. 494 29. 402 1. 00 20. 23 B	C
ATOM	8659 O PRO	359	112. 221 50. 683 29. 465 1. 00 22. 01 B	O
ATOM	8660 N SER	360	113. 474 48. 953 30. 163 1. 00 19. 33 B	N
ATOM	8661 CA SER	360	114. 212 49. 725 31. 160 1. 00 18. 75 B	C
ATOM	8662 CB SER	360	115. 122 48. 806 31. 968 1. 00 20. 74 B	C
ATOM	8663 OG SER	360	116. 163 48. 286 31. 149 1. 00 26. 03 B	0
ATOM	8664 C SER	360	115. 060 50. 841 30. 560 1. 00 18. 77	C
ATOM	8665 O SER	360	115. 410 50. 806 29. 382 1. 00 17. 99 B	0
ATOM	8666 N GLU	361	115. 394 51. 824 31. 393 1. 00 18. 96 B	N
ATOM	8667 CA GLU	361	116. 199 52. 970 30. 978 1. 00 18. 11 B	C
ATOM	8668 CB GLU	361	115. 982 54. 159 31. 919 1. 00 16. 34 B	C
ATOM ATOM ATOM	8669 CG GLU 8670 CD GLU 8671 OE1 GLU	361 361 361	116. 654 54. 007 33. 269 1. 00 21. 67 B 115. 743 53. 431 34. 342 1. 00 27. 42 B	C C
ATOM	8672 OE2 GLU	361	115. 067 52. 408 34. 091 1. 00 28. 62 B 115. 710 54. 009 35. 453 1. 00 31. 11 B	0 0

	•	FIG. 4-178	(Continued)
ATOM 8687 ND ATOM 8688 CE ATOM 8689 NE ATOM 8690 C ATOM 8691 O ATOM 8692 N ATOM 8693 CA ATOM 8694 CB ATOM 8695 CG ATOM 8696 CD ATOM 8696 CD ATOM 8697 CD ATOM 8699 CE ATOM 8700 CZ ATOM 8701 C ATOM 8701 C ATOM 8702 O ATOM 8703 N ATOM 8704 CA ATOM 8705 CB ATOM 8706 OG1 ATOM 8707 CG2 ATOM 8707 CG2 ATOM 8707 CG2 ATOM 8707 CG2 ATOM 8708 C	HIS 363 HIS 364 PHE 365 THR 365 THR 365 THR 365 THR 365 THR 365	117.674 52.595 31.007 1.00 16.97 B 118.118 51.870 31.888 1.00 16.23 B 118.449 53.079 30.030 1.00 16.09 B 118.027 53.805 28.817 1.00 13.66 B 119.879 52.772 29.985 1.00 15.32 B 120.207 52.916 28.505 1.00 13.19 B 119.362 54.086 28.121 1.00 12.78 B 120.601 53.806 30.832 1.00 16.34 B 120.096 54.911 31.021 1.00 17.05 B 121.768 53.448 31.353 1.00 17.21 B 122.550 54.374 32.164 1.00 18.58 B 122.626 53.875 33.603 1.00 18.58 B 121.324 53.965 34.333 1.00 19.33 B 120.156 53.301 34.158 1.00 19.36 B 121.111 54.851 35.368 1.00 19.36 B 121.111 54.851 35.368 1.00 19.36 <td>C O N C C C C O N C C C C N C N C O N C C C C</td>	C O N C C C C O N C C C C N C N C O N C C C C
ATOM 8709 O ATOM 8710 N ATOM 8711 CA	THR 365 LEU 366 LEU 366	128.662 58.260 30.015 1.00 20.68 B 130.329 58.163 31.515 1.00 22.60 B 130.740 59.544 31.304 1.00 25.75 B	O N C
	LEU 366 LEU 366 LEU 366 LEU 366 LEU 366 LEU 366 ASP 367 ASP 367 ASP 367	132.053 59.831 32.039 1.00 29.32 B 132.172 59.429 33.516 1.00 34.01 B 132.442 57.920 33.631 1.00 33.57 B 133.316 60.210 34.162 1.00 34.78 B 130.909 59.900 29.824 1.00 26.20 B 130.317 60.871 29.349 1.00 26.53 B 131.709 59.115 29.102 1.00 24.26 B 131.964 59.369 27.682 1.00 23.63 B 133.232 58.636 27.214 1.00 23.47 B 133.230 57.158 27.582 1.00 25.27 B	C C C C C O N C C

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					F I	[G	. 4 -	180				(Cor	ntinued)
.=													
ATOM ATOM	8771 C 8772 C			373 373	118. 59 117. 2		48. 627 49. 238	27. 969 27. 563) 21.40) 21.67		C	
ATOM	8773 N			373	116.0		48. 389	27. 855		21.07		N	
ATOM	8774 C			373	120. 13		47.049	31. 928		18.77		Ĉ	
ATOM	8775 0) <u>[</u>	LYS	373	120.69	95	45.980	31.712		18.48	В	0	
ATOM	8776 N			374	119.0		47. 150	32. 709		17.06		N	
ATOM				374	118.4		45. 972	33. 332		15.88		C	
ATOM ATOM		:B 1 :G2 1	ILE :	374 374	117. 59 116. 99		46. 339 45. 076	34. 526) 14.58) 12.18		C C	
ATOM				374	118. 34		47. 101	35. 130 35. 591) 12.10) 15.07		C	
ATOM				374	117. 51	17	47. 505	36. 809		13.03		Č	
ATOM	8782 C			374	117.6		45. 244	32. 303		16.94		č	
ATOM	8783 0		ILE :	374	116.64	49	45.803	31. 795		17.41	В	0	
ATOM	8784 N		ILE :	375	117.97		44.008	31.978		18.50		N	
ATOM	8785 C		ILE :	375	117.17		43. 226	31.033		19.71	В	C	
ATOM ATOM	8786 C 8787 C	G2 I	ILE :	375 375	117.84		43.117	29.625		19.62	В	C	
ATOM		G2 1		375	118. 12 119. 12		44. 496 42. 298	29. 070 29. 706) 19.13) 21.23	B B	C C	
ATOM		D1 I	ILE :	375	119. 82		42. 129	28. 373		23.06	В	Č	
ATOM	8790 C		ILE :	375	116. 98		41.815	31. 579		20.44	В	Č	
ATOM	8791 0		ILE :	375	117.73	35	41.356	32.443		20.03	В	0	
ATOM	8792 N			376	115.96		41.128	31.078		21.14	В	N	
ATOM	8793 C			376	115.70		39. 771	31.516		21.95	В	C	
ATOM ATOM	8794 C 8795 O			376 376	114. 34 114. 02		39. 318 38. 054	31. 003 31. 539		21.55	В	C	
ATOM	8796 C			376	116. 80		38. 899	30.936		25.40 23.06	B B	0 C	
ATOM	8797 0			376	117. 23		39. 127	29. 807		24.16	В	0	
ATOM	8798 N			377	117. 28		37. 914	31.698		24.67	В	N	
ATOM	8799 C		ASN 3	377	118.35	8	37.053	31.218	1.00	25.07	В	C	
ATOM	8800 CI		ISN 3	377	119. 43		36. 891	32.302		23.49	В	C	
ATOM	8801 C			377	119.01		35. 971	33. 444		23.86	В	C	
ATOM ATOM		D1 A D2 A		377 377	117. 95 119. 84		35. 340 35. 884	33. 397		23.70	В	0	
ATOM	8804 C			377	117.89		35. 681	34. 474 30. 736		20.11 26.79	B B	N C	
ATOM	8805 0			377	116. 70		35. 382	30. 699		28. 58	В	0	
ATOM	8806 N			378	118.86		34. 856	30. 353		29.97	B	N	
ATOM	8807 C			378	118.60		33.504	29.871	1.00	33.15	В	C	
ATOM	8808 CI			378	119.91		32.716	29.870		37.08	В	C	
ATOM	8809 CC			378	120.69		32. 870	31. 181		43.78	В	C	
ATOM ATOM	8810 CI 8811 OF			378 378	121.68 121.22		31.740	31. 427 31. 725		46.56	В	C	
ATOM		E2 G		378	121. 22		30. 613 31. 981	31. 321		47. 52 47. 91	B B	0 0	
ATOM	8813 C			78	117. 58		32. 760	30. 722		33. 63	В	Č	
ATOM	8814 0	G	LU 3	378	116.68		32. 113	30. 192		35. 16	B	ŏ	
ATOM	8815 N			379	117.74	0	32. 842	32.041	1.00	32.70	В	N	
ATOM	8816 CA			379	116. 83		32.160	32. 953		30. 44	В	C	
ATOM	8817 CF			79	117.54		31.806	34. 256		34. 46	В	C	
ATOM ATOM	8818 CC 8819 CI			379 379	117.84			34. 412		39.45	B B	C	
AT UIU	0013 (1	<i>y</i> G	იი ე	10	116.57	1	29. 475	34. 492	1.00	43. 32	D	C	

									(Continued)
				FIC	3. 4·	183			(00000000000000000000000000000000000000
ATOM	8918			130.576	51.416			В	С
ATOM	8919			129.879	51.713			В	0
ATOM	8920		390	131.349	52. 227			В	0
ATOM	8921	C ASP	390	128.887	48. 106			В	C
ATOM	8922		390	128.589	47. 557			В	0
ATOM ATOM	8923			129.081	47. 427			В	N
ATOM ATOM	8924 8925		391	128.967	45. 977			В	C
ATOM	8926	CB LYS	391 391	129. 981	45. 409			В	C
ATOM	8927	CD LYS	391	131.416	45. 724			В	C
ATOM	8928	CE LYS	391	132. 428 133. 816	45. 397			В	C
ATOM	8929	NZ LYS	391	133. 810	45. 911 45. 719	21. 112	1.00 55.62	В	C
ATOM	8930	C LYS	391	127. 550	45. 535	22. 192 20. 163	1.00 56.68 1.00 45.76	В	N
ATOM	8931	0 LYS	391	126.857	46. 191	20. 103	1.00 45.76	В	C
ATOM	8932	N LYS	392	127. 125	44. 419	19. 576	1.00 40.28	В	O N
ATOM	8933	CA LYS	392	125. 772	43. 916	19. 782	1.00 45.02	B B	N C
ATOM	8934	CB LYS	392	125. 218	43. 382	18. 458	1.00 46.84	В	C C
ATOM	8935	CG LYS	392	124. 750	44. 494	17. 529	1.00 49.00	В	C
ATOM	8936	CD LYS	392	124. 282	43. 970	16. 186	1.00 50.10	В	Č
ATOM	8937	CE LYS	392	123. 533	45.057	15. 436	1.00 51.49	B	č
ATOM	8938	NZ LYS	392	124. 298	46.338	15.419	1.00 52.49	B	Ň
ATOM	8939	C LYS	392	125. 529	42.895	20.886	1.00 43.84	B	Ċ
ATOM	8940	0 LYS	392	124. 386	42.512	21.134	1.00 44.15	B	0
ATOM	8941	N ASP	393		42.446	21.555	1.00 41.92	В	N
ATOM	8942	CA ASP	393		41.489	22.632	1.00 40.21	В	C
ATOM	8943	CB ASP	393		40. 268	22. 470	1.00 41.22	В	C
ATOM ATOM	8944 8945	CG ASP	393		39. 509	21. 194	1.00 41.43	В	C
ATOM	8946	OD1 ASP OD2 ASP	393		39. 350	20. 824	1.00 40.27	В	0
ATOM	8947	C ASP	393 393		39.062	20. 569	1.00 43.49	В	0
ATOM	8948	0 ASP	393		42. 158	23. 953	1.00 38.67	В	C
ATOM	8949	N CYS	394	127.818	42. 588	24. 188	1.00 39.07	В	0
ATOM	8950	CA CYS	394		42. 252 42. 870	24.816	1.00 35.47	В	N
ATOM	8951	C CYS	394		41.796	26. 117 27. 069	1.00 32.02 1.00 29.62	В	C
ATOM	8952	0 CYS	394		40.608	26. 787	1.00 29.02	В	C
ATOM	8953	CB CYS	394		43. 491	26. 639	1.00 23.41	B B	· C
ATOM	8954	SG CYS	394		42. 328	27. 301	1.00 31.32	В	S
ATOM	8955	N THR	395		42. 215	28. 193	1.00 26.53	В	N
ATOM	8956	CA THR	395		41. 279	29. 171	1.00 23.76	В	C
ATOM	8957	CB THR	395		41.493	29. 358	1.00 23.30	B	C
ATOM	8958	OG1 THR	395		41.265	28.115	1.00 25.56	B	ŏ
ATOM	8959	CG2 THR	395	129.518	40. 542	30.397	1.00 22.48	B	Č .
ATOM	8960	C THR	395		11.448	30.519	1.00 22.20	B	Č `
ATOM	8961	0 THR	395	126.707	12.556	31.035	1.00 23.25	B	Ŏ
ATOM	8962	N PHE	396	126.300	10. 354	31.095	1.00 19.02	В	N
ATOM	8963	CA PHE	396	125.658	10.444	32. 396	1.00 18.94	В	C
ATOM	8964	CB PHE	396		39. 206	32.652	1.00 17.62	В	Ċ
ATOM	8965	CG PHE	396		39. 225	31.918	1.00 19.32	В	С
ATOM	8966	CD1 PHE	396	122.477 4	0.112	32. 290	1.00 20.73	В	С

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					FIG. 4-184		(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8967 8968 8969 8970 8971 8972 8973 8974 8975 8976 8977 8980 8981 8982 8983 8984 8985 8986 8987 8988 8989	CE1 CE2 CZ C O N CA CB CG2 CG1 CD1 C O N CA CB OG1 CG2 C O N CA	ILE ILE THR THR THR THR THR THR LYS LYS	396 396 396 396 397 397 397 397 397 397 398 398 398 398 398 398	123. 265 38. 378 30. 837 1. 00 19. 67 121. 267 40. 157 31. 593 1. 00 20. 02 122. 062 38. 411 30. 130 1. 00 20. 02 121. 057 39. 303 30. 507 1. 00 22. 36 126. 712 40. 596 33. 488 1. 00 19. 09 127. 703 39. 866 33. 516 1. 00 21. 70 126. 511 41. 559 34. 380 1. 00 17. 18 127. 454 41. 774 35. 460 1. 00 14. 91 127. 819 43. 240 35. 566 1. 00 14. 47 128. 181 43. 762 34. 192 1. 00 14. 09 126. 644 44. 036 36. 135 1. 00 13. 14 126. 993 45. 472 36. 449 1. 00 11. 32 126. 885 41. 287 36. 791 1. 00 16. 82 127. 543 41. 376 37. 833 1. 00 18. 48 125. 651 40. 790 36. 753 1. 00 14. 86 124. 049 41. 255 38. 652 1. 00 14. 72 122. 968 41. 627 37. 784 1. 00 13. 55 124. 812 42	B B B B B B B B B B B B B B B B B B B	C C C C C C C C C C C C C C C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	8990 8991 8992 8993 8994 8995 8996 8997 8998 8999 9000 9001 9002 9003 9006 9007 9008 9009 9010 9011 9012 9013	CB CGC CD CE NZ CO N CA CB CG2 C CO N CA CB CG2 CCD2	LYS LYS LYS LYS LYS GLY GLY THR THR THR TRP TRP TRP	399 399 399 399 399 399 400 400 400 401 401 401 401 401 402 402 402 402 402 402	124.026 35.960 37.314 1.00 20.96 125.322 35.630 38.023 1.00 24.93 125.970 34.380 37.458 1.00 29.93 127.055 33.860 38.402 1.00 32.81 128.082 34.904 38.703 1.00 34.86 122.616 36.259 39.354 1.00 17.75 123.041 36.571 40.465 1.00 18.35 121.684 35.331 39.181 1.00 16.55 121.131 34.640 40.327 1.00 17.62 119.616 34.629 40.320 1.00 19.66 118.979 35.360 39.551 1.00 22.36 119.028 33.797 41.172 1.00 18.45 117.582 32.323 41.700 1.00 17.98 117.653 32.056 43.004 1.00 20.05 117.607 31.267 40.730 1.00 13.15 117.013 34.785 42.125 1.00 16.85	B B B B B B B B B B B B B B B B B B B	C C C C O N C C O C C O C C C C C C C C
ATOM ATOM	9014 9015	CE3	TRP TRP	402 402 402	121. 131 38. 164 42. 771 1. 00 18. 27 119. 504 39. 948 42. 542 1. 00 18. 13 119. 859 36. 453 43. 440 1. 00 16. 20	В В В	C C C

				•						(Continued)
					FIC	3. 4·	- 185	;		(Commueu)
ATOM	9016		1 TRP	402	121.143	36.842	43. 130	1.00 18.41	В	N
ATOM	9017		2 TRP	402	122.180	39.003			B	Ċ
ATOM	9018		3 TRP	402	120.553	40.784		1.00 18.56	B	Č
ATOM	9019		2 TRP	402	121.874	40.303	42.075		В	Č
ATOM	9020		TRP	402	116.827	38. 280			В	C
ATOM	9021		TRP	402	117. 439	38. 022			В.	0
ATOM	9022		GLU	403	116.309	39. 480			В	N
ATOM	9023			403	116. 368	40.554			В	C
ATOM	9024			403	114. 990	40.703		1.00 10.24	В	C
ATOM ATOM	9025			403	114. 408	39. 396	39. 398	1.00 10.20	В	C
ATOM	9026 9027			403	113. 288	39.607	38. 391	1.00 14.00	В	С
ATOM	9021		1 GLU 2 GLU	403	112.301	40.306	38. 713	1.00 15.50	В	0
ATOM	9029		GLU	403	113. 397	39.068	37. 271	1.00 14.63	В	0
ATOM	9030		GLU	403 403	116.852	41. 938	40.999	1.00 13.29	В	C
ATOM	9031	N	VAL	404	116.785	42.301	42.171	1.00 14.74	В	0
ATOM	9032	CA	VAL	404	117. 322 117. 800	42.716	40.031	1.00 12.89	В	N
ATOM	9033	CB	VAL	404	118. 926	44. 067 44. 420	40. 270	1.00 12.91	B.	C
ATOM	9034		I VAL	404	110. 320	45. 859	39. 265 39. 453	1.00 11.91	В	C
ATOM	9035	CG	VAL	404	120.096	43. 484	39. 459	1.00 13.92 1.00 8.31	В	C
ATOM	9036	C	VAL	404	116.607	44. 994	40. 039	1.00 8.31 1.00 14.23	B B	C
ATOM	9037	0	VAL	404	116. 129	45. 105	38. 918	1.00 14.23	В	C
ATOM	9038	N	ILE	405	116. 122	45. 653	41.089	1.00 10.13	В	O N
ATOM	9039	CA	ILE	405	114. 968	46.540	40.951	1.00 13.56	В	C
ATOM	9040	CB	ILE	405		47.020	42. 339	1.00 12.98	В	Č
ATOM	9041		ILE	405		47. 763	42. 183	1.00 7.46	В	Č
ATOM	9042		ILE	405		45.824	43. 282	1.00 14.03	В	Č
ATOM	9043		ILE	405		44.705	42.732	1.00 10.06	B	č
ATOM	9044	C	ILE	405		47.762	40.088	1.00 14.39	B	č
ATOM	9045	0	ILE	405		48.156	39. 226	1.00 14.58	. B	Ö
ATOM	9046	N	GLY	406		48.367	40.315	1.00 14.30	B	Ň
ATOM	9047	CA	GLY	406		49.521	39. 521	1.00 12.80	B	Ċ
ATOM	9048	C	GLY	406		49.967	39. 708	1.00 13.75	В	Č
ATOM	9049	0 N	GLY	406		49. 708	40. 737	1.00 16.89	В	0
ATOM ATOM	9050	N	ILE	407		50.618	38. 691	1.00 14.84	В	N
ATOM	9051 9052	CA CB	ILE	407	120. 161	51.144	38. 760	1.00 13.37	В	С
ATOM	9053		ILE	407	120. 797	51.192	37. 361	1.00 11.30	В	С
ATOM	9054	CC1	ILE ILE	407		52.077	37. 373	1.00 11.29	В	С
ATOM	9055	CD1		407		49. 768	36. 936	1.00 9.82	В	С
ATOM	9056	CDI	ILE	407 407		49. 545	35. 446	1.00 9.37	В	C
ATOM	9057	Õ	ILE	407 407	119.991	52. 546	39. 343	1.00 15.02	В	C
ATOM	9058	N	GLU	407	119. 236 120. 692	53. 361	38. 819	1.00 14.39	В	0
ATOM	9059	CA	GLU	408		52.825	40. 431	1.00 16.63	В	N
ATOM	9060	CB	GLU	408		54. 105 53. 849	41.105	1.00 18.23	В	<u>C</u> .
ATOM	9061	CG	GLU	408		52. 815	42.601	1.00 21.53	В	C
ATOM	9062	CD	GLU	408		53. 275	42. 906 42. 456	1.00 23.80	В	C
ATOM	9063	0E1	GLU	408		52. 429		1.00 27.87 1.00 30.29	В	C
ATOM	9064	OE2		408		54. 483	42. 598	1.00 30.29	B B	0
			0	100	114.016	77. 700	76.000	1.00 43.00	a	0

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					F I	G. 4-	186			(Continued)
ATOM	9065	С	GLU	408	121. 687	55. 094	40. 888	1.00 19.22	D	C
ATOM	9066	0	GLU	408	121. 067		40. 924		В	C
ATOM	9067	N	ALA	409	121. 400		40. 524	1.00 21.00	B B	0 N
ATOM	9068	CA	ALA	409	124. 048		40.473	1.00 18.30	В	N C
ATOM	9069	CB	ALA	409	124. 533		41.816	1.00 17.37	В	C
ATOM	9070	CD	ALA	409	125. 189		39. 755	1.00 10.18	В	C
ATOM	9071	ŏ	ALA	409	125. 323		39. 834	1.00 17.43	В	Ö
ATOM	9072	Ň	LEU	410	126.009		39.062	1.00 17.35	В	N
ATOM	9073	CA	LEU	410	127. 140	55.034	38. 311	1.00 17.53	B	Ċ
ATOM	9074	CB	LEU	410	126. 722		36. 857	1.00 16.60	B	č
ATOM	9075	CG	LEU	410	127.767		35. 862	1.00 18.12	B	č
ATOM	9076	CD1	LEU	410	128. 278		36.302	1.00 16.12	B	. Č
ATOM	9077	CD2	LEU	410	127.144		34.467	1.00 14.82	В	Č
ATOM	9078	C	LEU	410	128.356	55.969	38. 356	1.00 18.72	В	C
ATOM	9079	0	LEU	410	128. 228		38.190	1.00 20.28	В	0
ATOM	9080	N	THR	411	129. 532	55.396	38.589	1.00 18.37	. B	N
ATOM	9081	CA	THR	411	130. 786	56.142	38. 617	1.00 19.27	В	C
ATOM	9082	CB	THR	411	131.360		40.060	1.00 18.85	В	С
ATOM	9083	0G1	THR	411	131.869		40.514	1.00 17.72	В	0
ATOM	9084		THR	411	130. 284		41.012	1.00 17.11	В	C
ATOM	9085	C	THR	411	131.744		37. 784	1.00 20.67	В	C
ATOM	9086	0	THR	411	131.374	54. 200	37. 357	1.00 23.60	В	0
ATOM	9087	N	SER	412	132. 961	55. 772	37. 543	1.00 21.07	В	N
ATOM ATOM	9088 9089	CA CB	SER	412	133. 912	54. 988	36. 753	1.00 21.08	В	C
ATOM	9090	OG	SER SER	412 412	135. 124	55.827	36. 365	1.00 18.37	В	<u>C</u> .
ATOM	9091	C	SER	412	135. 926 134. 387	56. 086 53. 778	37.496	1.00 21.11	В	0
ATOM	9092	0	SER	412	134. 961	52. 843	37. 548 36. 995	1.00 22.07	В	C
ATOM	9093	N	ASP	413	134. 144	53. 790	38. 850	1.00 23.13 1.00 22.17	В	0 N
ATOM	9094	CA	ASP	413	134. 581	52.677	39.673	1.00 22.17	B B	N C
ATOM	9095	CB	ASP	413	135. 339	53. 198	40.895	1.00 25.67	В	C C
ATOM	9096	CG	ASP	413	136.731	53. 697	40.548	1.00 28.45	В	C
ATOM	9097		ASP	413	137. 338	54. 395	41.389	1.00 23.43	В	0
ATOM	9098		ASP	413	137. 228	53. 385	39. 444	1.00 29.95	В	Ö
ATOM	9099	С	ASP	413	133.446	51.777	40. 123	1.00 22.23	B	Č
ATOM	9100	0	ASP	413	133.624	50. 565	40. 248	1.00 22.67	. B	ŏ
ATOM	9101	N	TYR	414	132.274	52.362	40.351	1.00 21.41	B	Ň
ATOM	9102	CA	TYR	414	131.138	51.575	40.819	1.00 18.45	B	Ċ
ATOM	9103	CB	TYR	414	131.002	51.708	42.329	1.00 15.46	В	Č
ATOM	9104	CG	TYR	414	132. 101	51.071	43.131	1.00 14.79	В	C
ATOM	9105		TYR	414	132.118	49.699	43.357	1.00 14.59	В	C
ATOM	9106		TYR	414	133.093	49. 120	44.159	1.00 16.87	В	С
ATOM	9107		TYR	414	133.093	51.850	43.718	1.00 14.91	В	C
ATOM	9108		TYR	414	134.071	51. 282	44.512	1.00 16.48	В	С
ATOM	9109	CZ	TYR	414	134.066	49. 921	44. 733	1.00 16.25	В	C
ATOM	9110	OH	TYR	414	135.030	49. 369	45. 541	1.00 19.68	В	0
ATOM	9111	C	TYR	414	129. 787	51.898	40. 214	1.00 17.91	В	C
ATOM	9112	0	TYR	414	129. 547	52. 990	39.693	1.00 17.06	В	0
ATOM	9113	N	LEU	415	128. 901	50. 917	40. 323	1.00 16.46	В	N

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					FΙ	G. 4	- 188	}		(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	9163 9164 9165 9166 9167 9168 9170 9171 9172 9173 9174 9175 9178 9181 9182 9183 9184 9185 9186 9187 9188 9189 9190 9191 9192 9193 9194 9195 9196 9197 9198	ND C O N CA CB CC CD C C C C C C C C C C C C C C C	GLU GLU GLU GLU GLU GLU GLU GLU TYR TYR TYR TYR TYR TYR TYR TYR LYS LYS LYS LYS LYS GLY GLY GLY	420 420 421 421 421 421 421 421 421 421	115. 220 113. 072 116. 700 116. 135 118. 018 118. 895 120. 291 121. 358 122. 661 123. 169 123. 184 119. 028 119. 401 119. 386 119. 401 119. 386 121. 510 119. 198 121. 658 120. 813 121. 267 118. 401 117. 187 118. 933 117. 436 118. 393 117. 677 118. 692 117. 097 116. 114 117. 331 116. 430 114. 969 114. 102	40. 146 40. 818 40. 426 39. 368 40. 532 39. 393 39. 694 38. 747 38. 782 39. 890 37. 756 40. 023 39. 895 40. 746 40. 023 39. 895 40. 746 40. 023 39. 893 41. 334 41. 210 40. 488 40. 376 38. 779 37. 546 36. 486 36. 995 37. 278 37. 707 38. 595 37. 278 37. 707 38. 595 37. 278 37. 707 38. 595 37. 278 37. 707 38. 595 37. 278 37. 278	44. 193 44. 169 46. 638 46. 910 46. 543 46. 754	1.00 14.68 1.00 7.98 1.00 16.85 1.00 18.37 1.00 17.15	888888888888888888888888888888888888888	(Continued) 0 N C 0 N C 0 N C C C C C C C C C C C
ATOM ATOM	9201 9202	N CA	MET MET	425 425	114.695 113.322	37. 163 37. 627	49. 739 49. 968	1.00 20.34 1.00 18.53	B B	N C
ATOM ATOM ATOM ATOM	9203 9204 9205 9206	CB CG SD CE	MET MET MET MET	425 425 425 425	113. 234 113. 756 113. 506 111. 741	38. 329 37. 501 38. 352 38. 663	51. 317 52. 469 54. 020 53. 907	1. 00 19. 68 1. 00 22. 38 1. 00 24. 27 1. 00 21. 26	B B B	C C S
ATOM ATOM ATOM	9207 9208 9209	C O N	MET MET PRO	425 425 425 426	112. 908 113. 405 111. 968	38. 604 39. 725 38. 206	48. 871 48. 819 47. 999	1. 00 21. 26 1. 00 16. 75 1. 00 17. 33 1. 00 16. 64	B B B	C C O N
ATOM ATOM	9210 9211	CD CA	PRO PRO	426 426	111.173 111.530	36. 969 39. 089	48. 017 46. 910	1.00 17.29 1.00 15.29	B B	C C

		FΙ	G. 4-189)		(Continued)
ATOM 921 ATOM 922 ATOM 923 ATOM 9234 ATOM 9241 ATOM 9241 ATOM 9244 ATOM 9244 ATOM 9244	G CG PRO C GLY C ARG C A	F I 426	3 38. 233 46. 140 3 36. 823 46. 561 40. 379 47. 416 3 41. 402 46. 727 40. 321 48. 630 41. 480 49. 217 42. 449 49. 919 43. 462 50. 452 42. 144 49. 942 43. 036 50. 577 43. 771 49. 538 43. 363 48. 377 44. 844 49. 946 45. 630 49. 023 46. 667 48. 314 46. 947 46. 701 46. 279 45. 699 45. 008 45. 769 44. 227 46. 791 44. 520 44. 825 46. 328 49. 678 46. 983 50. 707	1. 00 15. 30 1. 00 15. 73 1. 00 15. 48 1. 00 15. 90 1. 00 14. 46	B B B B B B B B B B B B B B B B B B B	Continued) C C C C C O N C C C C O N C C C C C N C C C C
ATOM 9245 ATOM 9246 ATOM 9247	CB LEU 4 CG LEU 4 CD1 LEU 4	431 121. 709 431 122. 825 431 122. 501	50. 496 48. 713 51. 279 48. 012 51. 399 46. 528	1.00 16.67 1.00 18.10 1.00 17.30	B B B	C C C
ATOM 9248 ATOM 9249 ATOM 9250 ATOM 9251 ATOM 9252 ATOM 9253	C LEU 4 O LEU 4 N TYR 4 CA TYR 4	431 122. 998 431 122. 729 431 123. 367 432 123. 112 432 124. 344 432 124. 061	52.651 48.667 48.338 48.022 48.018 49.028 48.038 46.789 47.317 46.511 45.978 45.826	1. 00 14. 93 1. 00 17. 39 1. 00 19. 06 1. 00 17. 62 1. 00 18. 05 1. 00 17. 24	B B B B	C C O N C C
ATOM 9254 ATOM 9255 ATOM 9256 ATOM 9257 ATOM 9258 ATOM 9259 ATOM 9260	CG TYR 4 CD1 TYR 4 CE1 TYR 4 CD2 TYR 4 CE2 TYR 4 CZ TYR 4	432 123. 334 432 121. 962 432 121. 289 432 124. 015 432 123. 360 432 121. 996 432 121. 358	44. 944 46. 654 45. 034 46. 883 44. 049 47. 601 43. 843 47. 169 42. 862 47. 882 42. 968 48. 099 41. 994 48. 834	1. 00 18. 80 1. 00 19. 62 1. 00 19. 23 1. 00 17. 63 1. 00 18. 49 1. 00 20. 13 1. 00 21. 75	B B B B B	C C C C C

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					FIC	G. 4·	190			(Con	tinued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	9261 9262 9263 9264 9265 9266 9267 9268 9270 9271 9272 9273	C O N CA CB CCD CE NZ C O N CA	TYR TYR LYS	432 432 433 433 433 433 433 433 433 434 434	FIC 125. 193 124. 700 126. 474 127. 386 128. 237 129. 297 130. 239 131. 190 132. 101 128. 269 128. 654 128. 564 129. 411	48. 142 49. 066 47. 805 48. 460 49. 536 49. 022 50. 146 49. 723 50. 834 47. 343 46. 454 47. 364 46. 331		1. 00 17. 78 1. 00 18. 57 1. 00 16. 13 1. 00 14. 57 1. 00 16. 46 1. 00 16. 27 1. 00 16. 51 1. 00 16. 69 1. 00 17. 27 1. 00 13. 68 1. 00 11. 44 1. 00 13. 85 1. 00 15. 56	B B B B B B B B B B B B B B B B B B B	CON CON CCCC CCN CCON	tinued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	9274 9275 9276 9277 9278 9279 9280 9281 9282 9283 9284 9285	CB CG2 CG1 CD1 C O N CA CB CG CD OE1	ILE ILE ILE ILE ILE GLN GLN GLN GLN GLN	434 434 434 434 434 435 435 435 435 435	128. 645 128. 054 129. 580 128. 978 130. 646 130. 554 131. 804 133. 045 134. 253 135. 490 136. 715 136. 763	45. 504 46. 429 44. 458 43. 676 46. 973 48. 003 46. 374 46. 907 46. 264 47. 145 46. 461 46. 154	41. 124 40. 061 40. 518 39. 379 41. 573 40. 915 41. 809 41. 263 41. 956 41. 958 42. 547 43. 741	1. 00 14. 45 1. 00 11. 95 1. 00 14. 14 1. 00 14. 42 1. 00 16. 13 1. 00 17. 71 1. 00 18. 33 1. 00 20. 88 1. 00 21. 76 1. 00 24. 28 1. 00 25. 69 1. 00 26. 08	B B B B B B B B	0 C C C C C O N C C C C O	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	9286 9287 9288 9289 9290 9291 9292 9293 9294 9295 9296 9297		GLN GLN GLN LEU LEU LEU LEU LEU LEU LEU SER	435 435 436 436 436 436 436 436 436 437	137. 713 133. 068 132. 969 133. 200 133. 197 133. 050 131. 785 131. 748 130. 572 134. 391 134. 294 135. 517	46. 220 46. 617 45. 465 47. 668 47. 527 48. 905 49. 596 51. 035 48. 831 46. 790 46. 242 46. 775	41. 705 39. 767 39. 348 38. 965 37. 513 36. 880 37. 386 36. 920 36. 895 36. 908 35. 810 37. 613	1. 00 24. 68 1. 00 20. 60 1. 00 20. 57 1. 00 21. 54 1. 00 23. 39 1. 00 21. 46 1. 00 19. 80 1. 00 19. 31 1. 00 18. 85 1. 00 25. 55 1. 00 27. 46 1. 00 26. 98	B B B B B B B B	N C O N C C C C C O N	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	9298 9299 9300 9301 9302 9303 9304 9305 9306 9307	CA CB OG C O N CA CB CG OD1 OD2 C	SER SER SER SER ASP ASP ASP ASP	437 437 437 437 437 438 438 438 438 438 438 438	136. 690 137. 967 137. 940 136. 593 137. 152 135. 882 135. 704 136. 702 136. 622 135. 517 137. 659 134. 286	46. 069 46. 683 46. 694 44. 597 43. 736 44. 310 42. 930 42. 588 41. 135 40. 557 40. 575 42. 691	37. 119 37. 689 39. 102 37. 507 36. 832 38. 595 39. 049 40. 151 40. 571 40. 495 40. 990	1.00 26.89 1.00 26.26 1.00 31.19 1.00 27.29 1.00 29.17 1.00 26.66 1.00 26.32 1.00 28.65 1.00 30.81 1.00 32.19 1.00 33.46 1.00 24.90	B B B B B B B B	C C C C C C C C C C C C C C C C C C C	

										(Continued)
					FI	G. 4	- 191			(0011011101000
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	9310 9311 9312 9313 9314 9315 9316 9317 9318 9319 9320 9321 9322 9323 9324	CD2 CE2 CZ OH C O N	TYR TYR TYR TYR TYR TYR TYR TYR	439 439 439 439 439 439 439 439 439 439	133. 959 133. 461 132. 083 131. 301 131. 357 131. 420 131. 442 131. 322 131. 348 131. 405 131. 410 131. 928 130. 882 132. 953	43. 060 42. 046 41. 780 41. 243 42. 125 43. 514 44. 329 41. 572 42. 379 43. 753 44. 552 40. 823 40. 801 40. 030	40. 700 38. 753 39. 123 37. 924 36. 698 36. 814 35. 687 35. 416 34. 285 34. 430 33. 314 40. 294 40. 933 40. 584	1. 00 22. 15 1. 00 23. 79 1. 00 23. 74 1. 00 22. 94 1. 00 22. 91 1. 00 22. 44 1. 00 22. 19 1. 00 22. 08 1. 00 21. 13 1. 00 21. 92 1. 00 24. 24 1. 00 24. 38 1. 00 25. 27 1. 00 24. 21	B B B B B B B B B B B B B B B B B B B	(Continued) 0 N C C C C C C C C C N
ATOM ATOM ATOM ATOM	9325 9326 9327 9328	CA CB OG1 CG2 C	THR THR THR THR THR	440 440 440 440 440	132. 858 134. 102 135. 221 134. 418 132. 712	39. 094 38. 196 38. 975 37. 568 39. 852	41. 699 41. 806 42. 250 40. 462 43. 014	1.00 23.35 1.00 23.70 1.00 22.70 1.00 23.82 1.00 22.79	B B B B	C C O C C
ATOM ATOM ATOM ATOM ATOM	9329 9330 9331 9332 9333	O N CA CB CG	THR LYS LYS LYS LYS	440 441 441 441 441	132. 169 133. 200 133. 123 134. 396	39. 328 41. 087 41. 905 42. 741	43. 987 43. 039 44. 243 44. 375	1.00 21.81 1.00 22.86 1.00 22.90 1.00 25.86	B B B	O N C C
ATOM ATOM ATOM ATOM	9334 9335 9336 9337	CD CE NZ C	LYS LYS LYS LYS	441 441 441 441	135. 620 136. 871 138. 053 139. 319 131. 881	41. 878 42. 702 41. 804 42. 577 42. 794	44. 682 44. 878 45. 201 45. 346 44. 329	1.00 30.20 1.00 34.36 1.00 37.32 1.00 40.04 1.00 21.89	B B B B	C C C N C
ATOM ATOM ATOM ATOM ATOM	9338 9339 9340 9341 9342	O N CA CB CG1	LYS VAL VAL VAL VAL	441 442 442 442 442	131. 828 130. 880 129. 624 128. 458 127. 123	43. 891 42. 289 42. 984 42. 093 42. 770	43. 768 45. 039 45. 242 44. 799 45. 119	1.00 21.84 1.00 19.62 1.00 17.69 1.00 17.33 1.00 15.79	B B B B	O N C C C
ATOM ATOM ATOM ATOM ATOM	9343 9344 9345 9346 9347	CG2 C O N CA	VAL VAL VAL THR THR	442 442 442 443 443	128. 586 129. 502 129. 742 129. 129	41. 792 43. 299 42. 437 44. 528	43. 306 46. 733 47. 572 47. 066	1. 00 11. 20 1. 00 20. 40 1. 00 22. 84 1. 00 20. 64	B B B	C C O N
ATOM ATOM ATOM ATOM	9348 9349 9350 9351	CB OG1	THR THR THR THR	443 443 443 443	129. 015 130. 040 131. 370 129. 923 127. 641	44. 927 46. 035 45. 566 46. 442 45. 475	48. 461 48. 801 48. 546 50. 255 48. 819	1.00 22.17 1.00 24.13 1.00 28.90 1.00 22.91 1.00 23.06	B B B B	C C O C
ATOM ATOM ATOM ATOM ATOM	9352 9353 9354 9355 9356	O N CA C	THR CYS CYS CYS CYS	443 444 444 444 444	127. 210 126. 948 125. 656 125. 963 126. 866	46. 483 44. 835 45. 368 46. 516 46. 411	48. 254 49. 754 50. 163 51. 115 51. 941	1.00 26.29 1.00 21.88 1.00 22.22 1.00 20.79 1.00 19.89	B B B B	O N C C
ATOM ATOM	9357 9358	CB SG	CYS CYS	444 444	124. 801 123. 137 UBSTITUTE	44. 328 44. 986	50. 878 51. 221	1.00 24.50 1.00 27.42	B B	C S

			FIG. 4-192	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	9360 CA LE 9361 CB LE 9361 CB LE 9362 CG LE 9363 CD1 LE 9365 C LE 9366 O LE 9367 N SE 9368 CA SE 9369 CB SE 9370 OG SE 9371 C SE 9372 O SE 9372 O SE 9374 CA CYS 9375 C CYS 9376 O CYS 9377 CB CYS 9377 CB CYS 9378 SG CYS 9379 N GLU 9380 CA GLU 9381 CB GLU 9381 CB GLU 9381 CB GLU 9382 CG GLU 9381 CB GLU 9385 OE2 GLU 9386 C GLU 9387 CA LEU 9390 CB LEU 9391 CG LEU 9392 CD1 LEU 9393 CD2 LEU 9394 C LEU 9395 O LEU 9397 CA ASN 9397 CA ASN 9398 CB ASN	445 445 445 445 445 446 446 446 446 446	125. 205 47. 602 51. 005 1. 00 20. 20 125. 442 48. 785 51. 824 1. 00 17. 71 125. 651 49. 988 50. 899 1. 00 15. 76 126. 714 49. 756 49. 812 1. 00 15. 86 126. 930 51. 008 48. 970 1. 00 13. 93 128. 007 49. 333 50. 480 1. 00 12. 34 124. 333 49. 099 52. 814 1. 00 19. 64 124. 446 50. 036 53. 608 1. 00 20. 41 123. 262 48. 314 52. 776 1. 00 21. 11 122. 131 48. 552 53. 656 1. 00 20. 24 120. 947 49. 077 52. 834 1. 00 20. 38 120. 577 48. 143 51. 829 1. 00 18. 25 121. 708 47. 307 54. 411 1. 00 20. 86 121. 085 47. 404 55. 463 1. 00 21. 91 122. 043 46. 141 53. 874 1. 00 23. 84 120. 881 44. 602 56. 739 1. 00 24. 50 121. 845 44. 816 56. 004 1. 00 23. 42 122. 134 43	B C C C C C C C C C C C C C C C C C C C
ATOM	9398 CB ASN	450	118. 958 48. 731 61. 344 1. 00 23. 73 B	
ATOM ATOM	9399 CG ASN 9400 OD1 ASN	450 450	118. 226 48. 632 62. 661 1. 00 26. 67 B	C
ATOM ATOM	9401 ND2 ASN 9402 C ASN	450	118.199 49.733 63.406 1.00 26.73 B	O N
ATOM	9403 0 ASN	450 450	118. 772 46. 400 60. 469 1. 00 22. 01 B 117. 649 46. 701 60. 072 1. 00 21. 48 B	C
ATOM ATOM	9404 N PRO 9405 CD PRO	451	119. 215 45. 134 60. 442 1. 00 21. 65 B	O N
ATOM	9405 CD PRO 9406 CA PRO	451 451	120. 506 44. 673 60. 969 1. 00 20. 73 B 118. 430 44. 004 59. 941 1. 00 21. 39 B	C
ATOM	9407 CB PRO	451	118. 430 44. 004 59. 941 1. 00 21. 39 B 119. 362 42. 817 60. 162 1. 00 19. 94 B	C C

					P.C. 4	1 0 0		(Continued)
					FIG. 4-1	193		
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	9408 9409 9410 9411 9412 9413 9414 9415 9416 9417 9418 9420 9421 9422 9423 9424 9425	O C O N CA CB CC CD NE CZ NH	PRO PRO GLU GLU GLU GLU GLU GLU GLU ARG	451 451 452 452 452 452 452 452 452 453 453 453 453 453 453	117. 035 43. 774 6 116. 125 43. 392 5 116. 850 44. 003 6 115. 539 43. 767 6 115. 650 43. 767 6 116. 621 42. 720 6 116. 666 42. 675 6 117. 355 41. 782 6 116. 019 43. 529 6 114. 543 44. 867 6 113. 374 44. 582 6 115. 010 46. 101 6 114. 132 47. 198 6 113. 714 49. 685 6 113. 364 52. 058 6 113. 582 53. 245 6 114. 579 53. 391 63	31. 290 1. 00 21. 78 30. 509 1. 00 23. 49 59. 774 1. 00 25. 06 61. 800 1. 00 24. 25 62. 394 1. 00 32. 21 64. 455 1. 00 39. 54 65. 976 1. 00 47. 19 66. 627 1. 00 46. 89 61. 968 1. 00 25. 59 61. 733 1. 00 27. 44 61. 848 1. 00 23. 36 61. 478 1. 00 21. 67 2. 234 1. 00 21. 94 1. 872 1. 00 17. 23 2. 375 1. 00 16. 99 2. 927 1. 00 17. 21 3. 791 1. 00 17. 27	B B B B B B B B B B B B B B B B B B B	Continued) C C C C C C C C C C C C C C C C C C
ATOM ATOM	9428 9429	NH: C	ARG ARG	453 453	112.813 54.280 62	2.619 1.00 14.66	В	N
ATOM	9430	0	ARG	453	113.024 47.910 59	9. 994 1. 00 21. 78 9. 477 1. 00 20. 58	B B	C 0
ATOM ATOM	9431 9432	N	CYS	454	115. 206 47. 368 59	9.312 1.00 21.64	В	Ň
ATOM	9433	CA C	CYS CYS	454 454		7. 903 1. 00 19. 87	В	C
ATOM	9434	Õ	CYS	454 454		6.896 1.00 19.70 6.865 1.00 21.81	В	C
ATOM	9435	ČВ	CYS	454		6.865 1.00 21.81 7.770 1.00 19.47	B B	0 C
ATOM	9436	SG	CYS	454		3. 650 1. 00 18. 98	В	S
ATOM	9437	N	GLN	455		3. 051 1. 00 19. 11	В	N N
ATOM	9438	CA	GLN	455	114.692 45.305 55	5. 015 1. 00 14. 77	B	Ċ
ATOM	9439	CB	GLN	455	113. 881 44. 085 55	5. 457 1. 00 13. 34	B	č
ATOM ATOM	9440 9441	CG CD	GLN GLN	455 455		5. 711 1. 00 12. 92	В	C
ATOM	9442		GLN	455 455	113.425 42.482 57 112.514 41.958 56	7. 387 1. 00 13. 33	В	C
ATOM	9443		GLN	455		5. 749 1. 00 14. 25 3. 688 1. 00 13. 47	В	0
ATOM	9444	C	GLN	455		3. 669 1. 00 14. 10	B B	N C
ATOM	9445	0	GLN	455		704 1.00 14.35	В	0
ATOM	9446	N	TYR	456	113.803 47.094 53	5.597 1.00 13.95	В	N
ATOM	9447	CA	TYR	456		. 355 1. 00 13. 75	B	Ĉ
ATOM ATOM	9448 9449	CB CG	TYR	456		. 387 1. 00 13. 55	В	C
ATOM	9450		TYR TYR	456 456		. 045 1. 00 10. 86	В	C .
ATOM	9451		TYR	456		. 436 1. 00 10. 75	В	C
ATOM	9452		TYR	456		. 236 1. 00 9. 29 . 405 1. 00 9. 71	В	C
ATOM	9453		TYR	456		. 200 1. 00 4. 15	B B	C C
ATOM	9454	CZ	TYR	456		. 629 1. 00 8. 20	В	C
ATOM	9455	OH	TYR	456		. 464 1. 00 11. 71	В	0
ATOM	9456	С	TYR	456		. 190 1. 00 14. 04	·B	č

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			FIG. 4-195	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	9507 CA LY 9508 CB LY 9509 CG LY 9510 CD LY	\$\\ \text{463} \\ \text{463} \\ \text{463} \\ \text{463} \\ \text{463} \\ \text{463} \\ \text{464} \\ \text{464} \\ \text{464} \\ \text{464} \\ \text{464} \\ \text{465} \	124. 708 64. 736 43. 128 1. 00 22. 99 B 125. 109 64. 846 41. 728 1. 00 25. 69 B 125. 483 66. 291 41. 401 1. 00 27. 00 B 124. 275 67. 189 41. 270 1. 00 30. 44 B 124. 427 68. 146 40. 097 1. 00 35. 16 B 123. 083 68. 756 39. 718 1. 00 37. 88 B 123. 169 69. 566 38. 471 1. 00 40. 00 B 126. 204 63. 904 41. 230 1. 00 26. 63 B 126. 057 63. 297 40. 169 1. 00 27. 72 B 127. 305 63. 777 41. 959 1. 00 27. 45 B 128. 355 62. 868 41. 502 1. 00 28. 40 B 129. 710 63. 576 41. 429 1. 00 31. 19 B 130. 079 64. 030 40. 027 1. 00 35. 17 B 129. 200 66. 229 40. 022 1. 00 41. 38 B 128. 371 64. 817 38. 557 1. 00 38. 51 B 127.	
ATOM ATOM	9542 CD1 TYR 9543 CE1 TYR	467 467	128. 201 64. 119 49. 451 1. 00 25. 30 B	C C
ATOM ATOM	9544 CD2 TYR	467	127. 981 63. 095 51. 604 1. 00 26. 01 B	C C
ATOM	9545 CE2 TYR 9546 CZ TYR	467 467	129. 079 63. 811 52. 064 1. 00 26. 37 B 129. 736 64. 681 51. 206 1. 00 26. 55 B	С
ATOM	9547 OH TYR	467	129. 736 64. 681 51. 206 1. 00 26. 55 B 130. 841 65. 369 51. 645 1. 00 26. 89 B	C 0
ATOM	9548 C TYR	467	125. 428 60. 500 48. 584 1. 00 22. 16 B	C
ATOM ATOM	9549 O TYR 9550 N TYR	467	125. 034 60. 557 47. 420 1. 00 22. 32 B	0
ATOM	9550 N TYR 9551 CA TYR	468 468	124. 775 59. 840 49. 534 1. 00 21. 72 B	N
ATOM	9552 CB TYR	468	123. 492 59. 208 49. 251 1. 00 21. 47 B 123. 650 57. 817 48. 614 1. 00 19. 80 B	C
ATOM	9553 CG TYR	468	104 /00 = - = =	C
ATOM	9554 CD1 TYR.	468	124. 468 56. 797 49. 380 1. 00 19. 37 B 125. 844 56. 683 49. 184 1. 00 20. 24 B	C C

										(Continued)
				`•	FΙ	G. 4	- 196	5		(Convinuou)
ATOM ATOM	9555 9556		1 TYR 2 TYR		126. 588 123. 856				B B	C C
ATOM	9557		2 TYR		124. 588				В	Č
ATOM	9558				125.951				В	č
ATOM	9559				126.674	53.845			B	Ŏ
ATOM	9560		TYR		122.602				В	Ċ
ATOM	9561	0	TYR		123.068		51.588		B	0
ATOM	9562		GLN		121. 317	-		1.00 19.96	В	N
ATOM	9563				120. 369			1.00 18.78	В	C
ATOM	9564				119. 277				В	C
ATOM ATOM	9565 9566				118. 247			1.00 16.33	В	Ċ
ATOM	9567		GLN 1 GLN		117. 035			1.00 16.44	В	C
ATOM	9568		2 GLN		116. 438 116. 659			1.00 18.52	В	0
ATOM	9569	C	GLN		110.039			1.00 16.60	В	N
ATOM	9570	Õ	GLN	469	119. 353			1.00 18.75 1.00 20.25	В	C
ATOM	9571	Ň	LEU	470	119.641	57. 160	52. 359	1.00 20.25	B B	0 N
ATOM	9572	CA	LEU	470	119.013	55. 862	52. 383	1.00 16.05	В	N C
ATOM	9573	CB	LEU	470	119.871	54.860	53. 153	1.00 10.00	В	C
ATOM	9574	CG	LEU	470	120.920	54.116	52. 334	1.00 7.18	В	C
ATOM	9575		LEU	470	121.669	53.176	53. 230	1.00 9.83	B	č
ATOM	9576		2 LEU	470	120.248	53. 344	51.241	1.00 5.95	B	č
ATOM	9577	C	LEU	470	117.674	56.055	53.077	1.00 18.52	В	Č
ATOM	9578	0	LEU	470	117. 573	56. 769	54.082	1.00 17.50	В	0
ATOM ATOM	9579 9580	N	ARG	471	116.644	55. 437	52.517	1.00 20.97	В	N
ATOM	9581	CA CB	ARG ARG	471	115.306	55. 521	53.070	1.00 23.15	В	C
ATOM	9582	CG	ARG	471 471	114. 354 112. 907	56. 203	52.085	1.00 25.88	В	C
ATOM	9583	CD	ARG	471	111.997	56. 240 56. 927	52. 553 51. 541	1.00 31.75	В	C
ATOM	9584	NE	ARG	471	110.677	57. 213	52. 102	1.00 35.75 1.00 39.62	В	C
ATOM	9585	CZ	ARG	471	109.737	57. 920	51.478	1.00 39.02	B B	N
ATOM	9586	NH1		471	109.972	58. 412	50. 269	1.00 41.53	В	C N
ATOM	9587	NH2	ARG	471	108. 564	58. 142	52.063	1.00 40.93	В	N N
ATOM	9588	C	ARG	471	114.826	54.112	53. 345	1.00 24.13	В	C
ATOM	9589	0	ARG	471	114.604	53.323	52.425	1.00 25.84	·B	ŏ
ATOM	9590	N	CYS	472	114.687	53.796	54.621	1.00 23.64	B	Ň
ATOM	9591	CA	CYS	472	114. 219	52.487	55.042	1.00 23.00	В	C
ATOM	9592	C	CYS	472	112. 732	52.636	55. 321	1.00 21.14	В	C
ATOM ATOM	9593 9594	0 CD	CYS	472	112. 323	53. 547	56.036	1.00 21.12	В	0
ATOM	9595	CB SG	CYS CYS	472	114. 981	52.073	56. 299	1.00 23.91	В	C
ATOM	9596	N N	SER	$\begin{array}{c} 472 \\ 473 \end{array}$	114.149	50.907	57. 416	1.00 27.85	В	S
ATOM	9597	CA	SER	473	111.919	51.755	54. 756	1.00 19.44	В	N
ATOM	9598	CB	SER	473	110. 482 109. 789	51.846 52.191	54. 967 53. 646	1.00 18.92	В	C
ATOM	9599	0G	SER	473	110. 141	51. 261	53. 646 52. 642	1.00 18.36 1.00 21.93	В	C
ATOM	9600	Č	SER	473	109. 832	50.609	55. 581	1.00 21.93	B B	0
ATOM	9601	Ō	SER	473	108.615	50.465	55. 530	1.00 17.21	В	C 0
ATOM	9602	N	GLY	474	110.629	49.716	56. 156	1.00 16.48	В	N N
ATOM	9603	CA	GLY	474	110.055	48. 532	56. 771	1.00 16.90	B	C
										-

				(Continued)
	_		FIG. 4-197	
ATON Aton			111.040 47.425 57.091 1.00 16.48	ВС
ATON			112.149 47.403 56.563 1.00 18.05 110.643 46.446 57.913 1.00 16.25	B 0
ATOM			110.643 46.446 57.913 1.00 16.25 111.562 45.333 58.219 1.00 17.27	B N
ATOM	1 9608 CA PR	0 475	100 050 40 040	B C C
ATOM		0 475	100 445 44 005 50	B C
ATOM			110.896 44.680 59.411 1.00 14.77	B C
ATOM ATOM			109.012 47.214 59.716 1.00 14.52	B C
ATOM				B 0
ATOM				B N
ATOM	9615 C GLY		100 504 50 440 60 605	B C
ATOM	9616 O GLY	476	100 407 50 005 50 050	B C B O
ATOM			109. 454 51. 137 61. 748 1. 00 11. 74	B N
ATOM ATOM	9618 CA LEU		109. 222 52. 519 61. 331 1. 00 11. 92	B C
ATOM	9619 CB LEU 9620 CG LEU		109. 072 53. 412 62. 563 1. 00 10. 87	B C
ATOM	9621 CD1 LEU			B C
ATOM	9622 CD2 LEU		100 000 00 111	B C
ATOM	9623 C LEU		110 995 50 009 30 444	B C B C
ATOM	9624 O LEU		111 510 50 010 00 00	B C B 0
ATOM	9625 N PRO		109. 931 53. 894 59. 414 1. 00 13. 58	B N
ATOM ATOM	9626 CD PRO 9627 CA PRO	478	108. 541 54. 283 59. 121 1. 00 14. 52	B C
ATOM	9628 CB PRO	478 478		ВС
ATOM	9629 CG PRO	478	100 000 54 805 55 500	B C
ATOM	9630 C PRO	478	119 099 FF 100 F0 440	
ATOM	9631 O PRO	478	112. 033 55. 188 59. 118 1. 00 15. 11 111. 892 55. 820 60. 163 1. 00 16. 31	
ATOM	9632 N LEU	479	113. 197 55. 048 58. 490 1. 00 16. 04	
ATOM ATOM	9633 CA LEU 9634 CB LEU	479	114. 444 55. 621 58. 982 1. 00 15. 01 B	
ATOM	9634 CB LEU 9635 CG LEU	479 479	115. 279 54. 528 59. 657 1. 00 13. 83 B	
ATOM	9636 CD1 LEU	479	116. 675 54. 866 60. 179 1. 00 12. 46 116. 606 55. 990 61. 189 1. 00 13. 23	
ATOM	9637 CD2 LEU	479	117 960 E2 621 CO 010 + 00 + 0	
ATOM	9638 C LEU	479	117. 208 53. 631 60. 813 1. 00 12. 22 B 115. 204 56. 217 57. 801 1. 00 14. 97 B	•
ATOM	9639 O LEU	479	115. 395 55. 557 56. 783 1. 00 15. 80 B	
ATOM ATOM	9640 N TYR 9641 CA TYR	480	115.627 57.468 57.940 1.00 15.76 B	
ATOM	9641 CA TYR 9642 CB TYR	480	116. 350 58. 165 56. 883 1. 00 16. 51 B	- -
ATOM	9643 CG TYR	480 480	115. 631 59. 471 56. 517 1. 00 18. 80 B 114. 210 59. 293 56. 024 1. 00 20 33 B	С
ATOM	9644 CD1 TYR	480	119 010 50 804 71 001	C
ATOM	9645 CE1 TYR	480	113. 910 59. 364 54. 664 1. 00 22. 57 112. 604 59. 161 54. 196 1. 00 23. 68	C
ATOM	9646 CD2 TYR	480	113. 170 59. 019 56. 915 1. 00 20. 23 B	C C C C
ATOM ATOM	9647 CE2 TYR	480	111. 870 58. 815 56. 464 1. 00 22. 45 B	C
ATOM	9648 CZ TYR 9649 OH TYR	480	111. 591 58. 885 55. 102 1. 00 24. 15 B	č
ATOM	9650 C TYR	480 480	110. 312 58. 658 54. 648 1. 00 24. 41 B	0
ATOM	9651 0 TYR	480	117. 744 58. 483 57. 379 1. 00 15. 96 B 117. 910 59. 005 58. 482 1. 00 15. 89 B	C
ATOM	9652 N THR	481	117. 910 59. 005 58. 482 1. 00 15. 89 B 118. 743 58. 179 56. 559 1. 00 15. 76 B	0 N
			E 1-0 00.200 1.00 10.10 B	N

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			i		FIG	G. 4-	198			(Continued)
ATOM	9653	CA	THR	481	120. 129		56. 924	1.00 15.65	В	C
ATOM	9654	CB	THR	481	120.774		57. 480	1.00 14.54	В	C
ATOM	9655	0G1		481	120.459		56. 622	1.00 18.10	В	0
ATOM	9656		THR THR	481	120.256		58. 858	1.00 15.87	В	C
ATOM ATOM	9657 9658	C 0	THR	481 481	120.964 120.650		55. 752 54. 602	1.00 16.24 1.00 16.93	B B	C 0
ATOM	9659	N	LEU	482	120.030		56.058	1.00 16.93	В	N N
ATOM	9660	CA	LEU	482 482	122.033		55. 038	1.00 18.90	В	C
ATOM	9661	CB	LEU	482 482	123. 203	61.653	55. 279	1.00 19.21	B	C
ATOM	9662		LEU	482	123. 765	62. 439	54. 092	1.00 20.10	В	Č
ATOM	9663		LEU	482	122.736		52. 975	1.00 21.30	В	č
ATOM	9664		LEU	482	124. 115	63. 856	54. 525	1.00 22.66	B	č
ATOM	9665	C	LEU	482	124. 243	59. 373	55. 121	1.00 19.39	B	č
ATOM	9666	Ö	LEU	482	124.684		56. 210	1.00 20.79	B	Ŏ
ATOM	9667	Ň	HIS	483	124.849	59.096	53.970	1.00 18.33	B	Ň
ATOM	9668	CA	HIS	483	126.090	58. 332	53.903	1.00 16.79	B	Ċ
ATOM	9669	CB	HIS	483	125.791	56.894	53.488	1.00 14.55	В	C
ATOM	9670	CG	HIS	483	124.697		54.276	1.00 14.89	В	C
ATOM	9671		HIS	483	123.358		54. 264	1.00 15.13	В	C
ATOM	9672		HIS	483	124.933		55. 211	1.00 16.09	В	N
ATOM	9673		HIS	483	123. 788	54.867	55.736	1.00 13.84	В	C
ATOM	9674		HIS	483	122.816	55. 565	55.178	1.00 14.31	В	N
ATOM	9675	C	HIS	483	127.043		52.868	1.00 18.94	В	C
ATOM	9676	0	HIS	483	126.617	59.665	51.961	1.00 19.56	В	0
ATOM	9677	N	SER	484	128. 333	58. 645	53.003	1.00 19.52	В	N
ATOM	9678	CA	SER	484	129.318	59. 131	52.040	1.00 21.33	В	C
ATOM	9679	CB	SER	484	130. 520	59. 779	52. 738	1.00 21.77	В	C
ATOM	9680	OG C	SER	484	131.351	58. 803	53. 344	1.00 24.25	В	0
ATOM ATOM	9681 9682	C 0	SER SER	484 484	129.774	57. 907	51. 259	1.00 21.22	В	C
ATOM	9683	N	SER	485	129.942 129.979	56. 827 58. 076	49.960	- 1.00 19.26 1.00 22.12	В	0 N
ATOM	9684	CA	SER	485	130. 389	56. 967	49. 110	1.00 22.12	В	N C
ATOM	9685	CB	SER	485	130. 095	57. 301	47.645	1.00 25.02	B B	C C
ATOM	9686	OG		485	128. 715			1.00 30.40	В	Õ
ATOM	9687	Č	SER	485	131.840	56. 495	49. 221	1.00 26.33	В	Č
ATOM	9688	Ŏ	SER	485	132. 097		49. 138	1.00 27.23	В	ŏ
ATOM	9689	Ň	VAL	486	132. 781	57. 416	49. 407	1.00 28.07	B	Ň
ATOM	9690	CA	VAL	486	134. 194	57.056	49. 468	1.00 29.41	$\tilde{\mathbf{B}}$	Ĉ
ATOM	9691	CB	VAL	486	135.084		49.798	1.00 30.37	B	č
ATOM	9692	CG1	VAL	486	134. 786	58. 797	51.192	1.00 31.49	B	Č
ATOM	9693	CG2		486	136. 553	57.909	49.665	1.00 30.81	В	Č
ATOM	9694	C	VAL	486	134.507	55.929	50.442	1.00 30.57	В	Č
ATOM	9695	0	VAL	486	135. 269	55.016	50.119	1.00 31.62	В	0
ATOM	9696	N	ASN	487	133.922	55.979	51.630	1.00 30.95	В	N
ATOM	9697		ASN	487	134. 159	54. 928	52.610	1.00 31.75	В	С
ATOM	9698	CB	ASN	487	134.888	55. 498	53.833	1.00 35.87	В	С
ATOM	9699	CG		487	136. 336	55.868	53. 537	1.00 38.55	В	С
ATOM	9700	OD1		487	136. 838		54.014	1.00 38.47	В	0
ATOM	9701	ND2	ASN	487	137.019	55.026	52.759	1.00 37.49	В	N

					FIG	;. 4 -	- 199			(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	9702 9703 9704 9705 9706 9707 9708 9710 9711 9712 9713 9714 9715 9716 9717 9718 9719 9720	B O N CA CE CC OD OD CA CB CC	ASP ASP ASP ASP ASP ASP ASP LYS LYS LYS LYS LYS LYS LYS LYS LYS	487 487 488 488 488 488 488 488 489 489 489 489	132. 850 132. 830 131. 762 130. 449 130. 331 130. 253 129. 461 130. 977 130. 219 129. 654 130. 503 131. 607 131. 622 132. 805 132. 771 133. 883 129. 140 128. 556	54. 288 53. 486 54. 633 54. 108 52. 636 52. 440 53. 146 51. 572 54. 259 53. 382 55. 378 55. 610 56. 529 57. 898 58. 719 60. 133 60. 959 56. 216 56. 872 55. 968	53. 048 53. 982	1. 00 30. 74 1. 00 31. 45 1. 00 28. 68 1. 00 26. 66 1. 00 27. 90 1. 00 29. 72 1. 00 31. 30 1. 00 32. 18 1. 00 25. 72 1. 00 24. 30 1. 00 25. 25 1. 00 24. 10 1. 00 24. 94 1. 00 29. 19 1. 00 33. 11 1. 00 34. 94 1. 00 39. 70 1. 00 22. 29 1. 00 20. 15 1. 00 22. 04	B B B B B B B B B B B B B B B B B B B	C O N C C C O N C C C C N C O O C O O C O O C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	9722 9723 9724 9725 9726 9727 9728 9729 9730 9731 9732 9733 9734 9735	CA C O N CA CB CCD CD2 C O N CA CB	GLY GLY GLY LEU LEU LEU LEU LEU LEU LEU ARG ARG ARG	490 490 491 491 491 491 491 491 492 492 492	127. 352 127. 545 128. 091 127. 092 127. 234 127. 032 128. 153 127. 831 129. 441 126. 287 126. 735 124. 984 124. 020 124. 036	56. 487 57. 854 57. 989 58. 876 60. 233 61. 203 61. 167 62. 089 61. 577 60. 555 60. 780 60. 566 60. 881 62. 382	57. 657 58. 067 58. 676 59. 769 57. 965 58. 440 57. 283 56. 242 55. 090 56. 898 59. 586 60. 713 59. 316 60. 364 60. 644	1. 00 22. 04 1. 00 20. 03 1. 00 20. 18 1. 00 20. 54 1. 00 19. 44 1. 00 19. 54 1. 00 20. 53 1. 00 18. 39 1. 00 19. 23 1. 00 18. 31 1. 00 20. 91 1. 00 20. 73 1. 00 20. 73 1. 00 20. 06 1. 00 20. 71	B B B B B B B B B B B B B B B B B B B	N C O N C C C C C C C C C C C C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	9736 9737 9738 9739 9740 9741 9742 9743 9744 9745 9746 9747 9748 9749	C 0 N CA CB CG1	ARG ARG ARG ARG ARG ARG VAL VAL VAL VAL VAL VAL	492 492 492 492 492 492 493 493 493 493 493 493	123. 759 6 125. 193 6 125. 765 6 125. 022 6 127. 083 6 122. 585 6 122. 247 5 121. 746 6 120. 344 6 119. 883 5 118. 402 5 120. 698 5 119. 497 6	35. 192 35. 360 35. 286 30. 443 39. 998 30. 580 30. 211 39. 537 39. 215 38. 266	59. 625 58. 466 57. 380 58. 383 60. 085 58. 983 61. 107 61. 018 62. 325 62. 247 62. 574 60. 763	1.00 20.08 1.00 21.15 1.00 21.60 1.00 23.12 1.00 24.47 1.00 21.47 1.00 21.32 1.00 20.97 1.00 21.38 1.00 22.41 1.00 23.17 1.00 20.83 1.00 21.55 1.00 21.85	B B B B B B B B B B B B B B B B B B B	C C C C C C C C C C C C C C C C C C C

FIG. 4-201	(Continued)
ATOM 9801 C LEU 500 104.744 56.763 62.721 1.00 19.60 B ATOM 9802 C LEU 500 105.745 57.009 66.974 1.00 24.37 B ATOM 9803 N ASP 501 106.997 56.601 67.437 1.00 24.06 B ATOM 9805 CB ASP 501 107.301 55.392 67.868 1.00 26.06 B ATOM 9806 CG ASP 501 108.793 55.120 67.844 1.00 25.74 B ATOM 9807 OD1 ASP 501 109.145 53.848 68.556 1.00 26.66 B ATOM 9808 OD2 ASP 501 109.939 53.901 69.512 1.00 30.35 B ATOM 9809 C ASP 501 106.997 56.407 67.437 1.00 24.06 B ATOM 9807 OD1 ASP 501 109.145 53.848 68.556 1.00 26.66 B ATOM 9808 OD2 ASP 501 109.939 53.901 69.512 1.00 30.35 B ATOM 9809 C ASP 501 106.827 55.484 69.309 1.00 27.60 B ATOM 9810 O ASP 501 106.827 55.484 69.309 1.00 27.60 B ATOM 9811 N LYS 502 107.011 56.645 69.924 1.00 28.69 B ATOM 9812 CA LYS 502 107.034 58.184 71.834 1.00 33.97 B ATOM 9813 CB LYS 502 106.591 56.819 71.301 1.00 31.12 B ATOM 9816 CE LYS 502 106.591 56.819 71.301 1.00 31.12 B ATOM 9817 NZ LYS 502 106.597 59.822 73.766 1.00 36.56 B ATOM 9818 C LYS 502 106.599 59.822 73.766 1.00 36.56 B ATOM 9818 C LYS 502 106.599 59.822 73.766 1.00 33.97 B ATOM 9818 C LYS 502 106.597 59.822 73.766 1.00 33.97 B ATOM 9818 C LYS 502 106.597 59.99 71.301 1.00 31.12 B ATOM 9818 C LYS 502 106.597 59.99 71.301 1.00 33.97 B ATOM 9818 C LYS 502 106.597 59.822 73.766 1.00 33.97 B ATOM 9818 C LYS 502 106.597 59.822 73.766 1.00 33.97 B ATOM 9820 N MET 503 102.281 57.307 70.624 1.00 33.249 B ATOM 9821 CA MET 503 102.81 57.307 70.624 1.00 33.25 B ATOM 9822 CB MET 503 102.281 57.307 70.624 1.00 33.25 B ATOM 9823 CC MET 503 102.281 57.307 70.624 1.00 33.25 B ATOM 9824 SD MET 503 102.281 57.307 70.624 1.00 31.92 B ATOM 9830 CB LEU 504 102.471 53.993 68.836 1.00 30.00 B ATOM 9831 CD LEU 504 102.471 53.993 69.986 1.00 29.556 B ATOM 9832 CD LEU 504 102.471 53.993 69.986 1.00 29.556 B ATOM 9833 CD LEU 504 102.581 52.998 69.986 1.00 29.566 B ATOM 9834 C LEU 504 102.681 52.298 69.996 1.00 33.96 B	
ATOM 9840 CD GLN 505 106. 167 52. 836 72. 200 1. 00 42. 44 B ATOM 9841 OE1 GLN 505 106. 652 51. 408 71. 996 1. 00 43. 93 B ATOM 9842 NB9 GLN 505 107. 079 50. 746 72. 943 1. 00 45. 80 B	C C C O
ATOM 9844 O GLN 505 102. 375 52. 393 72. 960 1. 00 33. 38 B OATOM 9845 N ATOM 9845 N ATOM 9846 N ATOM	N C O
ATOM 9846 CA ASN 506 101.607 53.482 72.928 1.00 32.89 B	N C C

					· 	a 4				(Continued)
					F. 1 (G. 4-	,202		•	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	9849 9850 9851 9852 9853 9854 9855 9856 9857 9858 9859			506 506 506 506 507 507 507 507 507	101. 426 101. 703 99. 208 98. 058 99. 516 98. 497 98. 456 97. 287 98. 344 98. 717 99. 838	55. 608 56. 796 52. 933 52. 995 52. 305 51. 664 52. 293 51. 730 53. 811 50. 164 49. 676	75. 799 73. 903 72. 936 73. 377 71. 803 70. 974 69. 545 68. 755 69. 633 70. 825 70. 945	1. 00 41. 09 1. 00 39. 00 1. 00 30. 32 1. 00 30. 93 1. 00 26. 94 1. 00 25. 15 1. 00 23. 88 1. 00 21. 31 1. 00 22. 11 1. 00 25. 62 1. 00 26. 78	B B B B B B B B	0 N C O N C C C C C
ATOM	9860	N	GLN	508	97. 639	49. 432	70.567	1.00 25.89	B	N
ATOM	9861	CA	GLN	508	97. 730	47. 992	70.381	1.00 25.14	B	C
ATOM	9862	CB	GLN	508	96. 486	47. 281	70. 917	1.00 27.32	B	Č
ATOM	9863	CG	GLN	508	96. 322	47. 397	72. 422	1.00 29.65	B	C
ATOM	9864	CD	GLN	508	95. 190	46. 543	72. 958	1.00 30.81	B	C
ATOM	9865	OE1		508	95. 208	45. 312	72. 836	1.00 31.32	B	O
ATOM	9866	NE2		508	94. 199	47. 190	73. 561	1.00 29.92	B	N
ATOM	9867	C		508	97. 869	47. 740	68. 899	1.00 23.65	B	C
ATOM	9868	O	GLN	508	96. 944	47. 277	68. 241	1.00 22.60	B	O
ATOM	9869	N	MET	509	99. 046	48. 063	68. 385	1.00 23.78	B	N
ATOM	9870	CA	MET	509	99. 347	47. 895	66. 980	1. 00 23. 48	B	Č
ATOM	9871	CB	MET	509	100. 667	48. 578	66. 655	1. 00 23. 41	B	
ATOM	9872	CG	MET	509	100. 586	50. 070	66. 782	1.00 26.19	B	C
ATOM	9873	SD	MET	509	99. 279	50. 681	65. 719	1.00 28.03	B	
ATOM ATOM	9874 9875	CE C	MET MET	509 509	100. 207	50.994	64. 209	1.00 25.78	В	C C S C C
ATOM	9876	0	MET	509	99. 425 99. 902	46. 440 45. 599	66. 579 67. 343	1.00 23.44 1.00 24.15	B B	0
ATOM	9877	N	PRO	510	98. 951	46. 121	65. 365	1.00 22.69	B	N
ATOM	9878	CD	PRO	510	98. 308	47. 027	64. 395	1.00 22.87	B	C
ATOM	9879	CA	PRO	510	98. 974	44. 751	64. 854	1.00 21.97	B	C C
ATOM	9880	CB	PRO	510	97. 987	44. 807	63. 701	1.00 22.62	B	
ATOM ATOM	9881 9882	CG C	PRO PRO	510 510	100.381	46. 171 44. 434	63. 141 64. 379	1.00 22.72 1.00 21.20	B B	C ·
ATOM	9883	0	PRO	510	101. 249	45. 301	64. 353	1.00 19.97	B	O
ATOM	9884	N	SER	511	100. 605	43. 188	63. 997	1.00 22.07	B	N
ATOM	9885	CA	SER	511	101. 916	42. 782	63. 521	1.00 23.02	B	C
ATOM	9886	CB	SER	511	102. 481	41. 654	64. 392	1.00 23.03	B	C
ATOM	9887	OG	SER	511	101. 653	40. 500	64. 358	1.00 26.12	B	0
ATOM	9888	C	SER	511	101. 773	42. 299	62. 094	1.00 23.35	B	C
ATOM	9889	0	SER	511	100. 659	42.168	61.583	1.00 24.92	B	O
ATOM	9890	N	Lys	512	102. 906	42.035	61.458	1.00 22.83	B	N
ATOM	9891	CA	LYS	512	102. 916	41.556	60. 094	1.00 22.46	B	C
ATOM	9892	CB	LYS	512	103. 490	42.615	59. 168	1.00 21.81	B	C
ATOM	9893	CG	LYS	512	103. 494	42. 209	57. 705	1.00 23.24	B	C
ATOM	9894	CD	LYS	512	103. 820	43. 411	56. 851	1.00 24.28	B	C
ATOM	9895	CE	LYS	512	103. 824	43.080	55. 393	1.00 23.13	B	C
ATOM	9896	NZ	LYS	512	104. 160	44.299	54. 622	1.00 24.52	B	N
ATOM	9897	C	LYS	512	103. 742	40. 289	59. 993	1.00 22.87	B	Ċ

				FIG. 4-203	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	9898 9899 9900 9901 9902 9903 9904 9905 9907 9908 9909 9910 9911	N LYS CA LYS CB LYS CG LYS CD LYS CE LYS NZ LYS C LYS O LYS N LEU CA LEU CB LEU CG LEU CD1 LEU	513 513 513 513 513 513 513 514 514 514	FIG. 4 - 203 104.803	0 N C C C C C N C O N C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	9913 9914 9915 9916 9917 9918 9919 9920 9921 9922	CD2 LEU	514 514 514 515 515 515 515 515 515	100. 123 38. 790 53. 029 1. 00 19. 85 B 108. 438 39. 435 53. 701 1. 00 18. 42 B 106. 292 36. 132 55. 708 1. 00 24. 30 B 107. 123 35. 725 56. 519 1. 00 24. 87 B 105. 804 35. 361 54. 747 1. 00 25. 31 B 106. 233 33. 975 54. 634 1. 00 26. 30 B 105. 599 33. 156 55. 757 1. 00 28. 58 B 106. 403 31. 929 56. 108 1. 00 30. 08 B 107. 209 31. 474 55. 272 1. 00 31. 89 B 106. 216 31. 409 57. 224 1. 00 33. 36 B 105. 805 33. 414 53. 282 1. 00 26. 57 B	C C O N C C C O C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	9924 9925 9926 9927 9928 9929 9930 9931 9932 9933 9934	N PHE CA PHE CB PHE CCD PHE CD2 PHE CC1 PHE CE2 PHE CZ PHE C PHE C PHE O PHE	516 516 516 516 516 516 516 516 516 516	105. 940 32. 104 53. 103 1. 00 25. 46 B 105. 571 31. 496 51. 838 1. 00 25. 82 B 106. 792 31. 384 50. 930 1. 00 23. 83 B 107. 811 30. 395 51. 413 1. 00 22. 29 B 108. 896 30. 808 52. 176 1. 00 22. 68 B 107. 678 29. 042 51. 119 1. 00 21. 58 B 109. 836 29. 885 52. 642 1. 00 21. 89 B 108. 609 28. 113 51. 579 1. 00 21. 19 B 109. 689 28. 536 52. 342 1. 00 20. 70 B 104. 955 30. 117 51. 954 1. 00 26. 95 B 105. 063 29. 452 52. 980 1. 00 28. 94 B	0 N C C C C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	9935 9936 9937 9938 9939 9940 9941 9942 9943 9944 9945	N ILE CA ILE CB ILE CG2 ILE CG1 ILE CD1 ILE C ILE O ILE N ILE CA ILE CB ILE CG2 ILE	517 517 517 517 517 517 517 518 518 518 518	104. 307 29. 707 50. 872 1.00 27. 35 B 103. 697 28. 398 50. 755 1.00 28. 12 B 102. 155 28. 470 50. 729 1.00 26. 53 B 101. 645 29. 073 52. 016 1.00 27. 39 B 101. 682 29. 296 49. 537 1.00 27. 43 B 100. 175 29. 486 49. 486 1.00 26. 37 B 104. 202 27. 896 49. 411 1.00 30. 13 B 104. 575 28. 697 48. 551 1.00 29. 21 B 104. 239 26. 581 49. 228 1.00 33. 16 B 104. 709 26. 029 47. 969 1.00 36. 01 B 105. 680 24. 867 48. 190 1.00 36. 84 B 106. 133 24. 311 46. 845 1.00 36. 94 B	N C C C C C C C C C C

FIG. 4-204										(Continued)
ATOM ATOM	9947 9948		ILE ILE	518	106.884	25.349	49.000	1.00 38.21	В	C
ATOM	9949	CDI	ILE	518 518	107. 976 103. 558			1.00 40.77 1.00 37.38	B B	C C
ATOM	9950	0	ILE	518	102. 581	25.000			В	ŏ
ATOM	9951	N	LEU	519	103.679			1.00 39.11	В	N
ATOM ATOM	9952 9953	CA CB	LEU LEU	519	102.663			1.00 40.68	В	C
ATOM	9954	CG	LEU	519 519	101. 753 100. 989		44. 474 45. 612	1.00 39.71 1.00 39.82	B B	C C
ATOM	9955		LEU	519	100.051		45.045	1.00 39.32	В	C
ATOM	9956		LEU	519	100.194		46. 381	1.00 40.51	B	č
ATOM	9957	C	LEU	519	103. 388			1.00 42.22	В	C
ATOM	9958	0	LEU	519	104. 028			1.00 42.60	В	0
ATOM ATOM	9959 9960	N CA	ASN ASN	520 520	103. 299		43.419	1.00 43.53	В	N
ATOM	9961	CB	ASN	520 520	103. 963 103. 385		42. 285 40. 964	1.00 44.57 1.00 46.39	B B	C C
ATOM	9962	CG	ASN	520	102.045		40.639	1.00 48.97	В	C
ATOM	9963		ASN	520	101.168		41.498	1.00 50.54	B	ŏ
ATOM	9964		ASN	520	101.871	22. 312	39.386	1.00 50.46	В	N
ATOM	9965	Ç	ASN	520	105. 452		42.316	1.00 44.13	В	C
ATOM ATOM	9966 9967	0 N	ASN	520	106.004		41.348	1.00 44.64	B	0
ATOM	9968	N CA	GLU GLU	521 521	106. 097 107. 536		43. 431 43. 562	1.00 44.10 1.00 45.15	В	N C
ATOM	9969	CB	GLU	521	108. 272		42. 368	1.00 49.15	B B	C C
ATOM	9970	CG	GLU	521	109. 775		42. 339	1.00 54.49	В	č
ATOM	9971	CD	GLU	521	110.401	22. 274	41.004	1.00 58.04	B	Č
ATOM	9972		GLU	521	110. 307		40.597	1.00 59.07	В	0
ATOM	9973		GLU	521	110. 986		40.361	1.00 59.78	В	0
ATOM ATOM	9974 9975	C 0	GLU GLU	521 521	107. 922		43.661	1.00 42.18	В	C
ATOM	9976	N	THR	522	109. 034 107. 014		44. 072 43. 283	1.00 42.85 1.00 38.59	B B	0 N
ATOM	9977	CA	THR	522	107. 314		43. 333	1.00 34.63	В	N C
ATOM	9978	CB	THR	522	106. 605		42. 198	1.00 34.21	В	č
ATOM	9979		THR	522	107. 109	27. 115	40.936	1.00 34.20	$\tilde{\mathtt{B}}$	Õ
ATOM	9980		THR	522	106.866			1.00 33.69	В	С
ATOM ATOM	9981 9982	C 0	THR	522	106. 959	27. 441	44.664	1.00 32.83	В	C
ATOM	9983	N	THR Lys	522 523	106. 028 107. 727	27. 027 28. 464	45.350 45.011	1.00 32.75	В	0
ATOM	9984	CA	LYS	523	107. 559	29. 206	46. 245	1.00 31.06 1.00 29.30	B B	N C
ATOM	9985	CB	LYS	523	108. 940	29. 490	46. 838	1.00 29.00	В	Č
ATOM	9986	CG	LYS	523	108. 934	30. 329	48. 089	1.00 31.42	B	č
ATOM	9987	CD	LYS	523	110. 344	30. 567	48.607	1.00 32.07	В	Č
ATOM	9988	CE	LYS	523	111.045	29. 265	48. 943	1.00 33.13	В	C
ATOM ATOM	9989 9990	NZ C	LYS LYS	523 522	112. 388	29. 512	49. 545	1.00 35.72	В	N
ATOM	9991	0	LYS	523 523	106. 819 107. 256	30. 519 31. 335	45. 984 45. 173	1.00 28.56 1.00 29.36	B B	C
ATOM	9992	N	PHE	524	105. 692	30. 711	46. 661	1.00 25.30	В	O N
ATOM	9993	CA	PHE	524	104. 912	31.934	46. 517	1.00 22.61	В	C
ATOM	9994	CB	PHE	524	103. 529	31.637	45. 929	1.00 22.69	B	č
ATOM	9995	CG	PHE	524	103. 565	31. 136	44.516	1.00 21.75	В	C

FIG. 4-206										(Continued)
					r i	G. 4	200	•		
ATOM	10045	0	MET	528	100. 471			1.00 21.07	В	0
ATOM	10046	N	ILE	529	98. 432			1.00 19.01	В	N
ATOM ATOM	10047 10048	CA	ILE	529	98. 428			1.00 18.89	В	C
ATOM	10040	CB	ILE ILE	529 529	97.718			1.00 16.80	В	C
ATOM	10049		l ILE	529 529	97. 656 98. 469			1.00 13.98	В	C
ATOM	10050	CD1		529	99. 934		57. 296 57. 537	1.00 15.06 1.00 11.03	В	C
ATOM	10052	C	ILE	529	97. 656		60. 225	1.00 11.03	B B	C C
ATOM	10053	Õ	ILE	529	96. 457		60. 124	1.00 20.13	В	0
ATOM	10054	Ň	LEU	530	98. 359		61. 302	1.00 20.34	В	N N
ATOM	10055	CA	LEU	530	97. 717	39. 985	62. 420	1.00 21.13	В	Ç
ATOM	10056	CB	LEU	530	98.649		62. 976	1.00 19.85	В	č
ATOM	10057	CG	LEU	530	99.086		61.931	1.00 19.34	B	č
ATOM	10058		LEU	530	100. 238		62.461	1.00 20.33	В	Č
ATOM	10059		LEU	530	97. 897	37.010	61.562	1.00 19.04	В	C
ATOM	10060	C	LEU	530	97. 294		63. 521	1.00 22.34	В	C
ATOM	10061	0	LEU	530	98.006		63.854	1.00 23.45	В	0
ATOM	10062	N	PRO	531	96. 104		64. 088	1.00 23.19	В	N
ATOM	10063	CD	PRO	531	95. 105		63. 711	1.00 22.71	В	С
ATOM ATOM	10064 10065	CA	PRO	531	95. 600		65. 169	1.00 24.33	В	C
ATOM	10066	CB CG	PRO PRO	531	94. 188		65. 404	1.00 22.74	В	C
ATOM	10067	C	PRO	531 531	94. 276 96. 490		64.967	1.00 23.03	В	C
ATOM	10068	Õ	PRO	531	97. 244		66. 407 66. 562	1.00 25.18	В	C
ATOM	10069	Ň	PRO	532	96. 424		67. 300	1.00 24.64 1.00 26.64	B B	O N
ATOM	10070	CD	PRO	532	95. 502	43. 581	67. 326	1.00 25.36	В	C
ATOM	10071	CA	PRO	532	97. 246	42. 397	68. 513	1.00 27.91	В	C
ATOM	10072	CB	PRO	532	96.868	43. 698	69. 216	1.00 27.08	В	C
ATOM	10073	CG	PRO	532	95.443	43.897	68. 793	1.00 26.25	В	č
ATOM	10074	C	PRO	532	96.945	41.160	69.369	1.00 29.25	B	č
ATOM	10075	0	PRO	532	95.865	40.579	69.279	1.00 29.62	В	0
ATOM	10076	N	HIS	533	97.909	40.756	70.187	1.00 30.65	В	N
ATOM	10077	CA	HIS	533	97. 738	39.602	71.061	1.00 31.99	В	C
ATOM	10078	CB	HIS	533	96. 749	39. 945	72.172	1.00 32.50	В	C
ATOM	10079	CC	HIS	533	96. 981	41. 293	72. 783	1.00 35.12	В	C
ATOM ATOM	10080 10081		HIS	533	96. 168	42. 370	72.903	1.00 36.18	В	C
ATOM	10081		HIS HIS	533 533	98. 181 98. 096	41.653	73. 358	1.00 35.49	В	N
ATOM	10082		HIS	533	96. 885	42.892	73.807	1.00 36.37	В	Ç
ATOM	10084	C	HIS	533	97. 249	43. 350 38. 382	73. 544	1.00 37.01	В	N
ATOM	10085	Õ	HIS	533	96. 447	37. 590	70. 286 70. 791	1.00 33.21 1.00 32.78	В	C
ATOM	10086	N	PHE	534	97. 739	38. 243	69.058	1.00 32.78	В	0 NT
ATOM	10087	CA	PHE	534	97. 374	37. 125	68. 200	1.00 33.50	B B	N C
ATOM	10088	CB	PHE	534	98. 283	37. 085	66. 970	1.00 32.35	В	C
ATOM	10089	CG	PHE	534	97. 997	35. 942	66.041	1.00 32.06	В	Č
ATOM	10090	CD1	PHE	534	96.790	35. 871	65. 354	1.00 32.10	В	č
ATOM	10091	CD2		534	98. 936	34. 938	65. 848	1.00 32.66	B	č
ATOM	10092	CE1		534	96. 522	34.819	64. 486	1.00 31.59	B	č
ATOM	10093	CE2	PHE	534	98. 679	33.879	64. 982	1.00 32.91	В	Ċ

					•	(0 1)
					FIG. 4-207	(Continued)
ATOM				534	97. 469 33. 820 64. 298 1. 00 32. 93 B	С
ATOM			PHE	534	97. 503 35. 806 68. 941 1. 00 36. 77 B	C
ATOM			PHE	534	98. 532 35. 534 69. 565 1. 00 37. 84 B	0
ATOM			ASP	535	96. 463 34. 982 68. 868 1. 00 39. 07 B	N
ATOM	10098			535	96. 480 33. 680 69. 523 1. 00 40. 37 B	C
ATOM	10099			535	95. 458 33. 639 70. 655 1. 00 42. 55 B	C
ATOM	10100			535	95. 544 32. 363 71. 465 1. 00 45. 66 B	C
ATOM ATOM	10101		1 ASP	535	94. 783 32. 227 72. 445 1. 00 49. 45 B	0
ATOM	10102 10103		2 ASP	535	96. 372 31. 494 71. 125 1. 00 46. 59 B	0
ATOM	10103	C	ASP	535	96. 159 32. 601 68. 503 1. 00 39. 36 B	C
ATOM	10104	O N	ASP LYS	535 536	95. 047 32. 540 67. 996 1. 00 39. 17 B	0
ATOM	10106	CA		536	97. 135 31. 746 68. 216 1. 00 40. 23 B	N
ATOM	10107	CB		536	96. 964 30. 680 67. 233 1. 00 41. 20 B 98. 302 30. 001 66. 947 1. 00 42. 62 B	C
ATOM	10108	CG	LYS	536	00.000	C
ATOM	10109	CD	LYS	536	20 000	C
ATOM	10110	CE	LYS	536	20 201	C
ATOM	10111	NZ	LYS	536	99. 624 27. 800 64. 040 1. 00 48. 68 B 98. 648 26. 676 64. 079 1. 00 48. 77 B	C
ATOM	10112	C	LYS	536	95. 937 29. 620 67. 607 1. 00 40. 95 B	N C
ATOM	10113	0	LYS	536	95. 577 28. 785 66. 778 1. 00 41. 99 B	Ö
ATOM	10114	N	SER	537	95. 464 29. 649 68. 848 1. 00 40. 73 B	N
ATOM	10115	CA	SER	537	94. 469 28. 681 69. 296 1. 00 40. 33 B	Č
ATOM	10116	CB	SER	537	94. 598 28. 438 70. 805 1. 00 40. 23 B	č
ATOM	10117	0G	SER	537	94. 434 29. 636 71. 541 1. 00 40. 12 B	Ö
ATOM	10118	C	SER	.537	93.064 29.179 68.968 1.00 40.20 B	C
ATOM	10119	0	SER	537	92. 103 28. 412 68. 977 1. 00 40. 87 B	0
ATOM ATOM	10120	N	LYS	538	92. 951 30. 469 68. 674 1. 00 39. 23 B	N
ATOM	10121 10122	CA CB	LYS	538	91.666 31.067 68.337 1.00 37.32 B	C
ATOM	10122	CG	LYS LYS	538 538	91. 629 32. 517 68. 817 1. 00 39. 07 B	C
ATOM	10124	CD	LYS	538	92. 298 32. 747 70. 170 1. 00 41. 74 B 91. 534 32. 100 71. 316 1. 00 44. 86 B	Č .
ATOM	10125	CE	LYS	538	00 100 00 ==0	C
ATOM	10126	NZ	LYS	538	00 415 00 101	C
ATOM	10127	C	LYS	538	01 000 04 000 00 000	N
ATOM	10128	Ō	LYS	538	00 404 00 554 00 404	C
ATOM	10129	N	LYS	539	92. 464 30. 754 66. 101 1. 00 34. 33 B 90. 299 31. 288 66. 335 1. 00 33. 57 B	O N
ATOM	10130	CA	LYS	539	90. 038 31. 302 64. 895 1. 00 32. 92 B	C
ATOM	10131	CB	LYS	539	89. 049 30. 197 64. 510 1. 00 32. 99 B	C
ATOM	10132	CG	LYS	539	89. 736 28. 887 64. 143 1. 00 36. 07 B	č
ATOM	10133	CD	LYS	539	88. 757 27. 739 63. 893 1. 00 39. 32 B	č
ATOM	10134	CE	LYS	539	87. 720 28. 059 62. 816 1. 00 39. 62 B	č
ATOM	10135	NZ	LYS	539	86.644 28.969 63.310 ·1.00 39.49 B	Ň
	10136	C	LYS	539	89. 504 32. 666 64. 471 1. 00 31. 07 B	Ċ
	10137	0	LYS	539	88. 424 33. 087 64. 902 1. 00 30. 44 B	0
	10138	N	TYR	540	90. 274 33. 356 63. 633 1. 00 27. 48 B	N
	10139	CA	TYR	540	89. 893 34. 682 63. 165 1. 00 24. 82 B	C
	10140 10141	CB	TYR	540 540	91. 096 35. 624 63. 178 1. 00 23. 82 B	C
_		CG CD1	TYR	540 540	91. 849 35. 702 64. 482 1. 00 23. 61 B	C
• 111	10174	ועט	111/	540	92. 614 34. 627 64. 936 1. 00 21. 98 B	C

										(Continued)
					FIC	G. 4-	208			
ATOM	10143	CE1	TYR	540	93. 321	34. 708	66.130	1.00 21.65	В	С
ATOM	10144	CD2		540	91.810	36. 863	65.257	1.00 22.89	B	Ċ
ATOM	10145	CE2		540	92.507	36. 955	66.449	1.00 22.77	B	Č
ATOM	10146	CZ	TYR	540	93. 261	35. 875	66.881	1.00 22.87	B	Č
ATOM	10147	OH	TYR	540	93. 950	35. 965	68.062	1.00 23.97	B	Ö
ATOM	10148	C	TYR	540	89. 335	34. 694	61.749	1.00 23.62	В	č
ATOM	10149	ŏ	TYR	540	89.670	33. 842	60. 925	1.00 23.93	B	ő
ATOM	10150	N	PRO	541	88. 457	35. 660	61.452	1.00 21.89	B	Ň
ATOM	10151	CD	PRO	541	87. 820	36. 667	62.320	1.00 21.22	В	Ċ
ATOM	10152	CA	PRO	541	87.917	35. 719	60.095	1.00 20.52	B	č
ATOM	10153	CB	PRO	541	86.770	36. 717	60. 228	1.00 20.30	В	Č
ATOM	10154	CG	PRO	541	87. 243	37. 629	61.317	1.00 20.36	В	C C
ATOM	10155	C	PRO	541	89.077	36. 266	59. 276	1.00 19.86	В	č
ATOM	10156	ŏ	PRO	541	90.026	36. 799	59.841	1.00 19.00	В	ŏ
ATOM	10157	N	LEU	542	89. 028	36. 147	57.961	1.00 19.38	В	Ň
ATOM	10158	CA	LEU	542	90. 133	36. 655	57. 169	1.00 13.33	В	Č
ATOM	10159	CB	LEU	542	91.027	35. 483	56.741	1.00 18.21	В	Č
ATOM	10160	CG	LEU	542	92. 215	35. 768	55.816	1.00 10.30	В	Č
ATOM	10161		LEU	542	93. 296	34. 721	56.025	1.00 13.24	В	č
ATOM	10162		LEU	542	91. 741	35. 775	54.374	1.00 11.03	В	Č
ATOM	10163	C	LEU	542	89. 677	37. 458	55.954	1.00 13.31	В	Č
ATOM	10164	ŏ	LEU	542	88. 720	37. 087	55. 282	1.00 17.31	В	0
ATOM	10165	N	LEU	543	90. 368	38. 564	55.694	1.00 18.08	В	N N
ATOM	10166	CA	LEU	543	90. 075	39. 430	54. 559	1.00 14.81	В	C
ATOM	10167	CB	LEU	543	89. 816	40. 872	55.015	1.00 13.13	В	C ·
ATOM	10168	CG	LEU	543	89. 568	41.892	53.886	1.00 12.33	В	Č
ATOM	10169		LEU	543	88. 317	41. 497	53.113	1.00 13.11	В	C
ATOM	10170		LEU	543	89. 409	43. 294	54. 454	1.00 11.87	В	C
ATOM	10171	CDZ	LEU	543	91. 273	39. 415	53.620	1.00 11.31	В	C
ATOM	10172	ŏ	LEU	543	92. 349	39. 893	53.966	1.00 14.33	В	0
ATOM	10173	N	LEU	544	91. 091	38. 866	52. 428	1.00 14.04	В	
ATOM	10174	CA	LEU	544	92. 191	38. 807	51.480	1.00 15.02	В	N
ATOM	10175	CB	LEU	544	92. 006	37. 609	50. 539	1.00 16.19	В	C
ATOM	10176	CG	LEU	544	93. 163	37. 231	49.608	1.00 10.34	В	C
ATOM	10177		LEU	544	94. 345	36. 752	50. 429	1.00 14.33		
ATOM	10178		LEU	544	92. 713	36. 128	48.654	1.00 15.30	В	C
ATOM	10179	CDZ	LEU	544	92. 276	40. 109	50.679	1.00 15.79	В	C
ATOM	10113	ŏ	LEU	544	91.437	40. 103	49.819	1.00 10.49	B B	C
ATOM	10181	N	ASP	545	93. 280	40. 925	50.997	1.00 17.02	В	0 N
ATOM	10182	CA	ASP	545	93. 515	40. 323	50. 306	1.00 13.13		N
ATOM	10183	CB	ASP	545	94. 479				В	C
ATOM	10183	CG	ASP			43.069	51.117	1.00 15.71	В	C
ATOM	10184		ASP	545 545	94. 703	44. 434	50.483	1.00 15.88	B	C
ATOM	10186		ASP	545 545	94. 285	44.641	49. 324	1.00 14.36	В	0
ATOM	10180	C	ASP	545 545	95.304	45. 304	51.144	1.00 15.41	В	0
ATOM	10188	Ö	ASP	545 545	94. 175	41.757	49.004	1.00 14.61	В	C
ATOM	10189	N	VAL	545 546	95. 235	41.135	49.014	1.00 13.17	В	0 N
ATOM	10109	CA	VAL	546	93. 567	42.098	47.881	1.00 15.03	B	N
ATOM		CB	VAL		94.116	41.667	46.614	1.00 17.39	B B	C
VION	10191	CD	1 LT	546	93. 199	40. 579	46.014	1.00 19.44	D	С

		(Continued)								
					FIG	r. 4	209	l		
ATOM ATOM	10192 10193	3 CG	VAL VAL	546	93. 717 93. 109	40. 124 39. 410	46.983	1.00 17.87 1.00 20.93	B B	C C
ATOM ATOM	10194 10195		VAL VAL	546 546	94. 343 93. 601	42. 722 43. 694	45. 542 45. 447	1.00 17.09 1.00 18.12	В	C 0
ATOM	10196		TYR	547	95.391	42.519	44.745	1.00 15.70	В	N
ATOM ATOM	10197 10198			547 547	95. 670 96. 838	43. 378 44. 335	43. 595 43. 821	1.00 14.90 1.00 12.56	В	C
ATOM	10199			547		45. 241	42. 622	1.00 12.30	B B	C C
ATOM	10200			547	98.064	45.063	41.727	1.00 12.01	B	č
ATOM ATOM	10201 10202		1 TYR 2 TYR	547 547		45. 839	40.578	1.00 9.97	В	C
ATOM	10202		2 TYR	547		46. 226 47. 002	42. 331 41. 183	1.00 11.82 1.00 8.62	B B	C C
ATOM	10204	CZ	TYR	547		46. 804	40. 314	1.00 10.60	В	C
ATOM	10205			547		47. 573	39.179	1.00 12.10	В	0
ATOM ATOM	10206 10207		TYR TYR	547 547		42. 392 42. 205	42.485	1.00 13.60	В	C
ATOM	10208		ALA	548		41.763	41. 548 42. 608	1.00 13.39 1.00 13.66	B B	O N
ATOM	10209		ALA	548	97.594	40.730	41.672	1.00 14.14	В	Č
ATOM ATOM	10210 10211		ALA	548		39. 518	41.807	1.00 11.57	В	C
ATOM	10211	C 0	ALA ALA	548 548		41. 105 40. 234	40. 207 39. 340	1.00 13.67 1.00 14.21	В	C
ATOM	10213	N	GLY	549		42. 386	39. 913	1.00 14.21	B B	O N
ATOM	10214	CA	GLY	549	98.078	42.765	38. 524	1.00 12.26	В	Č
ATOM ATOM	10215 10216	C 0	GLY GLY	549 549		42. 209	38. 046	1.00 12.16	В	C
ATOM	10217	N	PRO	549 550		41. 717 42. 256	38. 855 36. 739	1.00 12.33 1.00 13.98	B B	O N
ATOM	10218	CD	PRO	550		42.760	35. 644	1.00 13.38	В	C
ATOM	10219	CA	PRO	550		41.736	36.217	1.00 13.32	B	C
ATOM Atom	10220 10221	CB CG	PRO PRO	550 550		42.007	34. 721	1.00 14.56	В	C
ATOM	10222	C	PRO	550 550		42.015 42.459	34. 473 36. 832	1.00 14.10 1.00 13.86	B B	C C
ATOM	10223	0	PRO	550		43. 683	36. 785	1.00 13.45	. В	0
ATOM ATOM	10224 10225	N	CYS	551		41.694	37. 405	1.00 14.79	В	N
ATOM	10226	CA CB	CYS CYS	551 551	104. 283 4 105. 035 4	12. 244 13. 139	38. 027 37. 036	1.00 15.51	В	C
ATOM	10227	SG	CYS	551		13. 567	37. 543	1.00 17.05 1.00 17.09	B B	C S
ATOM	10228	C	CYS	551	103.967	13. 018	39. 312	1.00 16.05	В	Č
ATOM ATOM	10229 10230	O N	CYS SER	551		13. 938	39. 702	1.00 15.36	В	0
ATOM	10231	CA	SER	552 552		12. 631 13. 268	39. 976 41. 229	1.00 15.15 1.00 14.65	В	N
ATOM	10232	CB	SER	552		3. 149	41. 425	1.00 14.03	B B	C C
ATOM	10233	OG C	SER	552	100.604 4	1.789	41.427	1.00 14.39	В	0
ATOM ATOM	10234 10235	C 0	SER SER	552 552			42.418	1.00 15.21	В	C
	10236	N	GLN	553			42. 273 43. 594	1.00 15.34 1.00 14.73	B B	0 N
ATOM	10237	CA	GLN	553		_	44. 794	1.00 14.73	В	C
	10238	CB	GLN	553	105.138 4	3.017	44. 892	1.00 13.21	В	C
	10239 10240	CCD	GLN GLN	553 553				1.00 15.05	В	C
111 (111	10440	·UD	GTIA	000	107. 359 4	2. 585	46.090	1.00 15.66	В	C

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FIG. 4-210											itinued)
	•				P I	G. 4	210				
ATOM	10241		GLN		107. 812		46.400	1.00 16.56	В	0	
ATOM	10242		GLN		108. 138		45. 773	1.00 15.50	В	N	
ATOM	10243	C	GLN		102.921		46.012	1.00 14.58	В	C	
ATOM ATOM	10244	0 N	GLN		103. 148		46. 434	1.00 14.77	В	0	
ATOM	10245 10246	N CA	LYS LYS	554 554	102.031		46.568	1.00 14.78	В	N	
ATOM	10240	CB	LYS	554 554	101.284 99.817		47. 754 47. 633	1.00 16.57	В	C	
ATOM	10248	CG	LYS	554 554	99.031		46.630	1.00 17.81 1.00 18.63	В	C	
ATOM	10249	CD	LYS	554 554	99.047		47. 000	1.00 18.05	B B	C C	
ATOM	10250	CE	LYS	554	98. 228		48. 261	1.00 18.33	В	C	
ATOM	10251	NZ	LYS	554	96.769		48. 035	1.00 13.33	В	N	
ATOM	10252	C	LYS	554	101.890		49. 024	1.00 16.05	В	Č	
ATOM	10253	0	LYS	554	101.424		50. 124	1.00 17.37	B	ŏ	
ATOM	10254	N	ALA	555	102.939		48.866	1.00 15.91	B	N	
ATOM	10255	CA	ALA	555	103.622		50.004	1.00 15.84	В	Ċ	
ATOM	10256	CB	ALA	555	103.656	39. 210	49.833	1.00 15.51	В	C	
ATOM	10257	C	ALA	555	105.041	41.246	50.142	1.00 14.91	В	C	
ATOM	10258	0	ALA	555	105.954		49. 539	1.00 15.57	В	0	
ATOM	10259	N	ASP	556	105. 233		50. 924	1.00 16.20	В	N	
ATOM	10260	CA	ASP	556	106. 571	42.854	51.134	1.00 16.65	В	C	
ATOM	10261	CB	ASP	556	106. 801	44. 085	50. 243	1.00 17.94	В	C	
ATOM	10262	CG	ASP	556	105. 750	45. 159	50. 430	1.00 19.95	В	C	
ATOM ATOM	10263 10264		ASP	556	105. 355	45. 429	51. 583	1.00 22.16	В	0	
ATOM	10265	C	ASP ASP	556 556	105. 327	45. 751	49.415	1.00 21.01	В	0	
ATOM	10266	0	ASP	556	106.862 106.046	43. 202	52. 597	1.00 16.87	В	C	
ATOM	10267	N	THR	557	100.040	42. 962 43. 762	53. 480 52. 847	1.00 15.15 1.00 17.93	В	0	
ATOM	10268	CA	THR	557	108. 443	44. 132	54. 200	1.00 17.93	B B	N	
ATOM	10269	CB	THR	557	109. 923	43. 826	54. 396	1.00 18.07	В	C	
ATOM	10270	0G1		557	110.687	44. 589	53. 454	1.00 20.98	В	0	
ATOM	10271		THR	557	110. 188	42. 358	54. 157	1.00 19.55	В	Č	
ATOM	10272	C	THR	557	108. 203	45.616	54. 531	1.00 17.89	B	č	
ATOM	10273	0	THR	557	108.776	46.151	55.479	1.00 16.94	B	ŏ	
ATOM	10274	N	VAL	558	107. 348	46.272	53.754	1.00 16.56	B	Ň	
ATOM	10275		VAL	558	107.049	47.682	53.964	1.00 14.93	В	C	
ATOM	10276	CB	VAL	558	106. 483	48. 302	52.676	1.00 14.99	В	C	
ATOM	10277		VAL	558	106.033	49. 733	52. 940	1.00 13.18	В	C	
ATOM	10278		VAL	558	107. 544	48. 247	51.568	1.00 13.02	В	C	
ATOM	10279	C	VAL	558	106.058	47. 921	55. 109	1.00 15.99	В	C	
ATOM	10280	0 N	VAL	558	105.060	47. 211	55. 238	1.00 13.36	В	0	
ATOM ATOM	10281 10282	N CA	PHE	559	106. 348	48. 923	55. 941	1.00 15.43	В	N	
ATOM	10283	CB	PHE PHE	559 550	105. 484	49. 269	57.069	1.00 14.56	В	C	
ATOM	10284	CG	PHE	559 559	106. 303 105. 469	49. 933	58.173	1.00 12.72	В	C	
ATOM	10285	CD1		559	105. 469	50. 504 49. 712	59. 282 60. 247	1.00 11.04	В	C	
ATOM	10286	CD2		559	105.056	51.833	60. 347 59. 244	1.00 10.65 1.00 12.10	B B	C	
ATOM	10287	CE1		559	103.000	50. 232	61.356	1.00 12.10	В	C C	
ATOM	10288	CE2		559	104. 251	52. 360	60. 252	1.00 10.43	В	C	
ATOM	10289		PHE	559	103. 855	51.554	61. 307	1.00 8.93	В	Č	
									~	•	

	FIG. 4-211	(Continued)
ATOM 10290 C PH ATOM 10291 O PH ATOM 10292 N AR ATOM 10293 CA AR ATOM 10294 CB AR ATOM 10295 CG AR ATOM 10296 CD AR ATOM 10297 NE AR ATOM 10297 NE AR ATOM 10298 CZ AR ATOM 10299 NH1 AR ATOM 10300 NH2 AR ATOM 10301 C AR ATOM 10301 C AR ATOM 10302 O AR ATOM 10303 N LEI ATOM 10304 CA LEI ATOM 10304 CA LEI	E 559 104.395 50.230 56.592 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00	4. 21 B C 4. 64 B O 3. 77 B N 4. 06 B C 2. 20 B C 1. 36 B C 0. 73 B C 3. 38 B N 4. 76 B C 0. 68 B N 6. 46 B N 6. 46 B N 6. 54 B O 6. 62 B N
ATOM 10305 CB LEU ATOM 10306 CG LEU ATOM 10307 CD1 LEU ATOM 10308 CD2 LEU ATOM 10309 C LEU ATOM 10310 O LEU ATOM 10311 N ASN ATOM 10312 CA ASN ATOM 10313 CB ASN ATOM 10314 CG ASN ATOM 10315 OD1 ASN	561 99.626 53.875 59.100 1.00 11 561 100.694 53.872 60.189 1.00 12 561 100.901 55.299 60.698 1.00 8 561 100.275 52.934 61.319 1.00 10 561 98.114 52.725 57.475 1.00 12 561 97.987 53.734 56.785 1.00 10 562 97.222 51.748 57.465 1.00 12 562 96.071 51.841 56.577 1.00 15 562 96.462 51.267 55.220 1.00 14 562 96.924 49.823 55.318 1.00 14	. 68 B C . 53 B C . 41 B C . 22 B C . 59 B C . 30 B O . 69 B N . 06 B C . 07 B C . 26 B C
ATOM 10316 ND2 ASN ATOM 10317 C ASN ATOM 10318 O ASN ATOM 10319 N TRP ATOM 10320 CA TRP ATOM 10321 CB TRP ATOM 10322 CG TRP ATOM 10323 CD2 TRP ATOM 10324 CE2 TRP ATOM 10325 CE3 TRP	562 96. 582 49. 157 56. 423 1. 00 11. 562 94. 818 51. 139 57. 086 1. 00 14. 562 94. 712 50. 793 58. 260 1. 00 16. 563 93. 872 50. 936 56. 178 1. 00 15. 563 92. 616 50. 281 56. 502 1. 00 15. 563 91. 770 50. 132 55. 244 1. 00 13. 563 90. 365 49. 719 55. 511 1. 00 15. 563 89. 623 48. 721 54. 804 1. 00 12. 563 88. 330 48. 684 55. 369 1. 00 13.	A 43 B N B C B C B C B C B C B C B C B C B C B C
ATOM 10326 CD1 TRP ATOM 10327 NE1 TRP ATOM 10328 CZ2 TRP ATOM 10329 CZ3 TRP ATOM 10330 CH2 TRP ATOM 10331 C TRP ATOM 10332 O TRP ATOM 10333 N ALA ATOM 10334 CA ALA ATOM 10335 CB ALA ATOM 10336 C ALA ATOM 10337 O ALA ATOM 10338 N THR	563 89. 927 47. 856 53. 745 1. 00 10. 563 89. 512 50. 237 56. 456 1. 00 13. 563 88. 289 49. 617 56. 373 1. 00 14. 563 87. 346 47. 816 54. 911 1. 00 13. 563 88. 951 46. 995 53. 290 1. 00 9. 563 87. 673 46. 980 53. 872 1. 00 12. 563 92. 880 48. 919 57. 119 1. 00 16. 563 92. 279 48. 562 58. 132 1. 00 15. 564 93. 790 48. 161 56. 515 1. 00 17. 564 94. 124 46. 841 57. 042 1. 00 17. 564 94. 585 46. 973 58. 489 1. 00 18. 564 94. 585 46. 973 58. 489 1. 00 18. 564 94. 256 46. 127 59. 320 1. 00 18. 565 95. 332 48. 037 58. 793 1. 00 17.	99 B C 03 B N 35 B C 50 B C 48 B C 18 B C 81 B O 44 B N 65 B C 15 B C 07 B C

, <u>.</u>					FI	G. 4-	212			(Continued)
ATOM	10339	CA	THR	565	95. 817		60. 159	1.00 17.29	В	С
ATOM	10340	CB	THR	565	96.626		60. 294	1.00 17.13	B	Č
ATOM	10341	0G1	THR	565	97.677		59.330	1.00 20.36	B	0
ATOM	10342		THR	565	97. 238		61.676	1.00 18.23	B	Č
ATOM	10343	C	THR	565	94.665		61.157	1.00 15.84	В	C
ATOM	10344	0	THR	565	94. 738		62.249	1.00 14.07	В	0
ATOM	10345	N	TYR	566	93.605		60.781	1.00 15.76	В	N
ATOM	10346	CA	TYR	566	92.455		61.664	1.00 17.74	В	C
ATOM	10347	CB	TYR	566	91.543		61.177	1.00 15.61	В	C C C C C
ATOM	10348	CG	TYR	566	90.067		61.311	1.00 17.40	В	С
ATOM	10349	CD1	TYR	566	89. 303		60.195	1.00 17.77	В	С
ATOM	10350	CE 1	TYR	566	87.947		60.310	1.00 15.12	В	C
ATOM	10351	CD2	TYR	566	89. 432	50.086	62.556	1.00 18.30	В	C
ATOM	10352	CE2	TYR	566	88.073	49.789	62.682	1.00 17.35	В	C .
ATOM	10353	CZ	TYR	566	87. 340	49.441	61.550	1.00 17.10	В	C
ATOM	10354	OH	TYR	566	86.005	49.137	61.662	1.00 17.63	В	0
ATOM	10355	C	TYR	566	91.667	47.899	61.777	1.00 19.12	В	C
ATOM	10356	0	TYR	56.6	91. 249	47.517	62.871	1.00 20.12	В	0
ATOM	10357	N	LEU	567	91.481	47. 211	60.654	1.00 19.08	В	N
ATOM	10358	CA	LEU	567	90. 735	45.959	60.648	1.00 19.66	В	C
ATOM	10359	CB	LEU	567	90.606	45.419	59. 223	1.00 18.00	В	C
ATOM	10360	CG	LEU	567	89. 728	46.252	58. 284	1.00 18.48	В	C
ATOM	10361		LEU	567	89. 735	45.628	56.889	1.00 19.22	В	C
ATOM	10362		LEU	567	88. 310	46.325	58.835	1.00 15.78	В	C
ATOM	10363	C	LEU	567	91. 355	44.898	61.544	1.00 20.80	В	C
ATOM	10364	0	LEU	567	90. 645	44.102	62.157	1.00 23.88	В	0
ATOM	10365	N	ALA	568	92.677	44.883	61.628	1.00 19.62	В	N
ATOM	10366	CA	ALA	568	93. 347	43.898	62.466	1.00 20.08	В	C
ATOM	10367	CB	ALA	568	94. 746	43.601	61.907	1.00 18.06	В	C
ATOM	10368	C	ALA	568	93. 451	44.362	63.924	1.00 20.52	В	C
ATOM	10369	0	ALA	568	93. 319	43.569	64.849	1.00 20.37	В	0
ATOM	10370	N	SER	569	93. 674	45.653	64. 128	1.00 20.79	В	N
ATOM	10371	CA	SER	569	93. 827	46. 182	65.474	1.00 21.75	В	C
ATOM	10372	CB	SER	569	94. 520	47. 545	65. 401	1.00 21.85	В	C
ATOM	10373	OG	SER	569	94. 546	48. 188	66.657	1.00 22.64	В	0
ATOM	10374	C	SER	569	92. 525	46. 297	66. 267	1.00 22.83	В	C
ATOM	10375	0	SER	569	92. 505	46.029	67.470	1.00 22.38	В	0
ATOM	10376	N	THR	570	91.444	46. 679	65.589	1.00 22.26	В	N
ATOM	10377	CA	THR	570	90. 153	46.862	66. 232	1.00 21.45	В	C
ATOM	10378	CB	THR	570	89. 512	48. 191	65. 797	1.00 19.91	В	C
ATOM	10379	0G1	THR	570	90. 349	49. 285	66. 188	1.00 21.12	В	0
ATOM	10380		THR	570	88. 143	48. 351	66. 430	1.00 17.96	В	C
ATOM	10381	C	THR	570	89. 132	45. 751	65.974	1.00 24.43	В	C
ATOM	10382	0 M	THR	570	88. 453	45. 301	66. 894	1.00 27.79	В	0
ATOM	10383	N	GLU	571	89. 001	45.317	64. 727	1.00 23.34	В	N
ATOM	10384	CA	GLU	571	88. 030	44. 280	64. 415	1.00 21.95	В	C
ATOM	10385	CB	GLU	571	87. 499	44. 481	62.998	1.00 22.83	В	C
ATOM	10386	CC	GLU	571	87.004	45.888	62. 709	1.00 24.63	В	C C
ATOM	10387	CD	GLU	571	85. 957	46. 357	63. 696	1.00 25.17	В	C

FIG. 4-213											
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	10389 10390 10391 10392 10393	OE C O N CA CB	ASN	571 571 571 571 572 572 572 572	85. 236 85. 834 88. 606 87. 903 89. 887 90. 539 89. 998 90. 523	45. 509 47. 580 42. 874 41. 887 42. 784 41. 491 40. 744 41. 303	63. 897 64. 554 64. 362		B B B B B	0 0 C 0 N C C C	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	10396 10397 10398 10399	OD: ND: C O N CA CB	I ASN 2 ASN ASN ASN ILE ILE ILE ILE	572 572 572 572 573 573 573	90. 053 91. 522 90. 347 90. 112 90. 445 90. 311 89. 509	42. 335 40. 634 40. 639 39. 436 41. 280 40. 604 41. 456	68. 035 68. 121 63. 806 63. 903 62. 645 61. 365 60. 382	1. 00 30. 34 1. 00 30. 31 1. 00 21. 12 1. 00 20. 16 1. 00 19. 59 1. 00 18. 06 1. 00 18. 14	B B B B B	O N C O N C C	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	10404 10405 10406 10407 10408 10409 10410	CG1 CD1 C O N CA CB	ILE ILE ILE ILE ILE ILE ILE ILE	573 573 573 573 573 574 574	89. 371 88. 143 87. 336 91. 706 92. 480 92. 038 93. 340 93. 724	40. 735 41. 778 42. 735 40. 425 41. 376 39. 216 38. 978 37. 494	59. 057 60. 970 60. 131 60. 777 60. 739 60. 337 59. 724 59. 740	1. 00 18. 53 1. 00 19. 49 1. 00 20. 04 1. 00 18. 47 1. 00 19. 08 1. 00 17. 57 1. 00 18. 02 1. 00 19. 09	B B B B B	C C C O N C C	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	10411 10412 10413 10414 10415 10416 10417 10418	CG1	ILE ILE ILE ILE ILE VAL VAL VAL	574 574 574 574 574 575 575		37. 280 37. 031 35. 553 39. 423 38. 981 40. 296 40. 777 42. 308	58. 870 61. 172 61. 282 58. 265 57. 500 57. 876 56. 498	1.00 20.13 1.00 21.02 1.00 20.47 1.00 17.84 1.00 19.48 1.00 17.13 1.00 16.42	B B B B B	C C C O N C	
ATOM ATOM ATOM ATOM ATOM ATOM	10419 10420 10421 10422 10423 10424 10425	CG1 CG2 C O N CA CB	VAL VAL VAL ALA ALA ALA	575 575 575 575 576 576 576	94. 271 93. 242 95. 452 96. 592 95. 186 96. 246 96. 062	42. 753 42. 948 40. 187 40. 488 39. 344 38. 683 37. 176	56. 430 54. 985 57. 261 55. 786 56. 124 54. 797 54. 056 54. 127	1. 00 16. 55 1. 00 16. 06 1. 00 15. 54 1. 00 16. 02 1. 00 16. 68 1. 00 16. 21 1. 00 15. 22 1. 00 12. 38	B B B B B B	C C C O N C C	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	10426 10427 10428 10429 10430 10431 10432 10433	C O N CA CB OG C	ALA SER SER SER SER SER SER SER	576 576 577 577 577 577 577	95. 397 97. 470 97. 722 98. 368 97. 456 98. 642	39. 117 39. 710 38. 811 39. 123 40. 495 41. 504 38. 045	52. 601 52. 046 51. 996 50. 606 50. 474 50. 866 50. 069	1.00 15.92 1.00 16.20 1.00 14.35 1.00 13.57 1.00 13.58 1.00 16.22 1.00 13.24	B B B B B	C O N C C C C	
ATOM ATOM ATOM	10434 10435 10436	N CA CB	PHE PHE PHE	578 578 578	98. 462 99. 262	37. 522 37. 712 36. 676 35. 407	50. 788 48. 800 48. 183 48. 079	1.00 13.05 1.00 11.98 1.00 11.24 1.00 11.42	B B B	O N C C	

					FIC	G. 4-	214	٠.		(Cor	tinued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	10437 10438 10439 10440 10441 10442 10443 10445 10446 10447 10448 10450 10451 10452 10453 10454 10455	CD2 CE1 CE2 CZ C O N CA CB CG OD1 OD2 C O N CA C	PHE PHE PHE PHE ASP ASP ASP GLY GLY ARG	578 578 578 578 578 578 579 579 579 579 579 579 579 580 580 580	99. 136 100. 196 98. 697 100. 805 99. 297 100. 354 99. 746 99. 002 101. 005 101. 617 103. 008 102. 957 102. 053 103. 816 101. 734 102. 633 100. 809 100. 838 101. 458 102. 269 101. 080	34. 232 33. 628 33. 679 32. 483 32. 537 31. 936 37. 096 37. 704 36. 780 37. 682 39. 090 39. 842 39. 451 35. 741 34. 927 35. 510 34. 274 34. 470 35. 376 33. 611	47. 481 48. 152 46. 280 47. 640 45. 762 46. 446 46. 805 46. 039 46. 516 45. 227 45. 401 45. 954 45. 954 45. 796 44. 488 44. 753 43. 570 42. 815 41. 450 41. 227 40. 521	1.00 10.60 1.00 10.29 1.00 10.36 1.00 11.15 1.00 11.72 1.00 10.56 1.00 10.76 1.00 11.14 1.00 9.94 1.00 9.15 1.00 13.00 1.00 14.87 1.00 11.19 1.00 11.60 1.00 12.07 1.00 10.77 1.00 11.96 1.00 13.34 1.00 12.96 1.00 14.18	B B B B B B B B B B B B B B B B B B B	CCCCCCONCCCOOCONCCON	itinued)
ATOM ATOM	10458 10459	CA CB	ARG ARG	581 581	101.615 101.085	33. 714 32. 570	39. 187 38. 338	1.00 15.34 1.00 13.67	B B	C	
ATOM ATOM ATOM	10460 10461 10462	CG CD NE	ARG ARG ARG	581 581 581	101. 809 101. 172 99. 980	31. 283 30. 076 29. 652	38. 666 38. 023 38. 740	1. 00 15. 30 1. 00 14. 62 1. 00 13. 01	B B B	C C	
ATOM ATOM	10463 10464	CZ	ARG ARG	581 581	99. 186 99. 467	28. 672 28. 024	38. 330 37. 207	1.00 13.01 1.00 13.69 1.00 13.99	B B	N C N	
ATOM ATOM	10465 10466	C	ARG ARG	581. 581	98. 112 101. 237	28. 348 35. 069	39. 036 38. 624	1.00 12.41 1.00 17.21	B B	N C	
ATOM ATOM ATOM	10467 10468 10469	O N CA	ARG GLY GLY	581 582 582	100. 175 102. 128 101. 868	35. 615 35. 628	38. 934 37. 817	1.00 17.96 1.00 18.14	B B	0 N	
ATOM ATOM	10470 10471	C C O	GLY GLY	582 582	102. 454 102. 557	36. 933 37. 998 39. 151	37. 258 38. 159 37. 754	1.00 17.73 1.00 16.81 1.00 18.98	В В В	C C 0	
ATOM ATOM	10472 10473	N CA	SER SER	583 583	102. 835 103. 423	37. 625 38. 588	39. 378 40. 309	1.00 15.90 1.00 16.60	B B	N C	
ATOM ATOM	10474	CB OG	SER SER	583 583	103. 437 104. 229	38. 024 36. 856	41.730	1.00 17.47 1.00 21.54	B B	0 0	
ATOM ATOM ATOM	10476 10477 10478	C O N	SER SER GLY	583 583 584	104. 841 105. 389 105. 441	38. 901 38. 176 39. 970	39. 841 39. 013 40. 359	1.00 15.56 1.00 17.79	B B	C 0	
ATOM ATOM	10479 10480	CA C	GLY GLY	584 584	106. 776 107. 969	40. 334 40. 158	39. 908 40. 831	1.00 14.64 1.00 13.05 1.00 12.28	B B B	N C C	
ATOM ATOM	10481 10482	0 N	GLY TYR	、584 585	107.851 109.129	39. 648 40. 583	41. 949 40. 325	1. 00 11. 78 1. 00 12. 34	B B	0 N	
ATOM ATOM ATOM	10483 10484 10485	CA CB CG	TYR TYR TYR	585 585 585	110. 412 110. 335 109. 704	40. 536 41. 383 42. 719	41. 034 42. 304 42. 047	1.00 12.19 1.00 11.93	B B B	C C C	
	100		~ ***	-	100.107	14.110	10. VT(1.00 12.41	Ŋ	U	

					FIC	1.	215			(Continued)
						. 4	. 410			
ATOM	10486		1 TYR	585		43.694		1.00 12.30	В	С
ATOM	10487		1 TYR	585		44. 891	40.979	1.00 12.43	В	C
ATOM	10488		2 TYR	585		42. 983		1.00 10.95	В	Č
ATOM ATOM	10489		2 TYR	585 585		44. 179		1.00 12.28	В	C
ATOM	10490 10491	CZ OH	TYR TYR	585 585		45. 126		1.00 13.31	В	C
ATOM	10491	С	TYR	585	107. 831	46. 306		1.00 14.33	В	0
ATOM	10493	0	TYR	585		39. 141	41.394	1.00 12.01	В	C
ATOM	10494	N	GLN	586		38. 979 38. 144	42. 319 40. 655	1.00 13.01	В	0
ATOM	10495	CA	GLN	586		36. 763	40. 906	1.00 11.45 1.00 11.62	В	N
ATOM	10496	CB	GLN	586		36. 071	40. 300	1.00 11.02	В	C
ATOM	10497	CG	GLN	586		36. 854	42. 867	1.00 10.30	B B	C C
ATOM	10498	CD	GLN	586		36. 533	43. 295	1.00 14.38	В	C
ATOM	10499		GLN	586		35. 452	43. 816	1.00 12.14	В	0
ATOM	10500		GLN	586		37. 478	43.060	1.00 15.36	В	N
ATOM	10501	C	GLN	586		36. 023	39.602	1.00 12.85	В	Č
ATOM	10502	0	GLN	586		34. 786	39. 574	1.00 13.97	B	ŏ
ATOM	10503	N	GLY	587		36. 778	38. 525	1.00 11.70	B	N
ATOM	10504	CA	GLY	587		36.168	37. 242	1.00 11.61	B	Ĉ
ATOM	10505	C	GLY	587	110.405	35.960	36.373	1.00 14.10	В	Č
ATOM	10506	0	GLY	587		35. 786	36.884	1.00 13.91	В	0
ATOM	10507	N	ASP	588		35. 949	35.054	1.00 16.19	В	N
ATOM	10508	CA	ASP	588		35. 776	34. 105	1.00 17.70	В	C
ATOM	10509	CB	ASP	588		35. 993	32. 680	1.00 18.98	В	C
ATOM	10510	CG	ASP	588		37. 312	32. 505	1.00 20.57	В	С
ATOM ATOM	10511 10512		ASP	588		88. 335	33. 040	1.00 23.28	В	0
ATOM	10512	C C	ASP ASP	588		37. 327	31.809	1.00 23.25	В	0
ATOM	10513	0	ASP	588 588		34. 454	34. 139	1.00 17.46	В	C
ATOM	10515	N	LYS	589		4. 389	33. 635	1.00 16.74	В	0
ATOM	10516	CA	LYS	589		3. 397 2. 143	34. 697 34. 734	1.00 18.02	В	N
ATOM	10517	CB	LYS	589		1.030	35. 372	1.00 20.00 1.00 22.21	В	C
ATOM	10518	CG	LYS	589		9. 710	35. 443	1.00 22.21	B B	C
ATOM	10519	CD	LYS	589		8. 579	35. 940	1.00 27.10	В	C C
ATOM	10520	CE	LYS	589		7. 273	36.111	1.00 33.79	В	Č
ATOM	10521	NZ	LYS	589		6. 232	36. 771	1.00 35.98	В	Ň
ATOM	10522	C	LYS	589		2.362	35. 536	1.00 20.94	B	Č
ATOM	10523	0	LYS	589		1.781	35. 242	1.00 23.79	B	Ŏ
ATOM	10524	N	ILE	590		3. 212	36. 552	1.00 18.06	В	N
ATOM	10525	CA	ILE	590		3. 523	37. 379	1.00 14.07	В	С
ATOM	10526	CB	ILE	590		3. 901	38. 814	1.00 11.33	В	C
ATOM	10527		ILE	590		4. 654	39. 538	1.00 9.61	В	C
ATOM	10528		ILE	590		2. 635	39. 585	1.00 10.89	. В	C
ATOM ATOM	10529		ILE	590		2. 888	40. 897	1.00 7.05	В	C
ATOM	10530 10531	C 0	ILE	590 500		4. 682	36. 753	1.00 15.70	В	C
ATOM	10532	N	ILE MET	590 591		4. 583	36.511	1.00 16.31	В	0
ATOM	10533	CA	MET	591		5. 774	36. 465	1.00 15.00	В	N
ATOM	10534	CB	MET	591		6. 948 8. 088	35. 907 35. 750	1.00 14.79	В	C
	-4001	₩.	1		JBSTITUTE S		35. 759 RULE 26)	1.00 14.22	В	С
						(,		

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					∘ F I	G. 4	216			(Continued)
ATOM ATOM	10535 10536	CG SD	MET MET	591 591	105. 854 107. 027	39.452	35. 581	1.00 18.55 1.00 17.84	B B	C S
ATOM ATOM	10537 10538	CE C	MET MET	591 591	107. 813 104. 788			1.00 16.39 1.00 14.86	В	C
ATOM	10539	0	MET	591	103. 643			1.00 14.80	B B	C 0
ATOM	10540	N	HIS	592	105. 451			1.00 14.66	В	N
ATOM ATOM	10541 10542	CA CB	HIS HIS	592 592	104. 863 105. 962		32. 343 31. 332	1.00 14.33 1.00 15.14	B B	C
ATOM	10543	CG	HIS	592	106. 753	36.626	30. 922	1.00 17.56	В	C C C C
ATOM ATOM	10544		HIS	592	106.626		31. 252	1.00 17.20	В	
ATOM	10545 10546		HIS HIS	592 592	107. 810 108. 300		30. 041 29. 845	1.00 17.84 1.00 16.59	B B	N C
ATOM	10547	NE 2	2 HIS	592	107. 598	38.620	30. 567	1.00 16.88	В	N
ATOM ATOM	10548 10549	0 0	HIS HIS	592	103.859		32. 355	1.00 15.17	В	C
ATOM	10550	N	ALA	592 593	103. 224 103. 708		31. 344 33. 500	1.00 15.89 1.00 15.86	B B	O N
ATOM	10551	CA	ALA	593	102. 775	32.810	33.615	1.00 14.02	B	Č
ATOM ATOM	10552 10553	CB C	ALA ALA	593 593	102. 690 101. 393		35.060	1.00 13.60	В	C
ATOM	10554	0	ALA	593	101. 593	33. 195 32. 335	33. 106 32. 631	1.00 15.66 1.00 17.83	B B	C 0
ATOM	10555	N	ILE	594	101.043	34.478	33. 207	1.00 16.63	В	Ň
ATOM ATOM	10556 10557	CA CB	ILE ILE	594 594	99. 731 99. 035	34. 945 35. 857	32. 745 33. 791	1.00 16.87	В	C
ATOM	10558		ILE	594	98. 506	35. 017	34. 932	1.00 15.87 1.00 16.36	B B	C C
ATOM	10559	CG1		594	100.006	36.915	34. 321	1.00 16.86	В	C
ATOM ATOM	10560 10561	CD1 C	ILE ILE	594 594	100. 533 99. 748	37. 882 35. 689	33. 274 31. 413	1.00 16.67	В	C
ATOM	10562	ő	ILE	594	98. 884	36. 525	31. 160	1.00 17.96 1.00 19.03	B B	C 0
ATOM	10563	N	ASN	595	100.718	35.385	30.558	1.00 17.93	В	N
ATOM ATOM	10564 10565	CA CB	ASN ASN	595 595	100. 802 102. 140	36. 050 35. 737	29. 263 28. 592	1.00 19.09 1.00 19.22	В	C
ATOM	10566	CG	ASN	5 9 5	102. 140	36. 441	27. 260	1.00 19.22	B B	C C
ATOM	10567	OD1		595	102.320	37.668	27. 198	1.00 19.01	В	0
ATOM ATOM	10568 10569	C	ASN ASN	595 595	102. 377 99. 659	35. 667 35. 641	26. 184 28. 330	1.00 19.95 1.00 19.09	В	N
ATOM	10570	0	ASN	595	99. 456	34. 460	28.076	1.00 19.09	B B	C 0
ATOM ATOM	10571 10572	N	ARG	596	98. 933	36.630	27.814	1.00 19.66	В	N
ATOM	10572	CA CB	ARG ARG	596 596	97. 799 98. 212	36. 406 35. 588	26. 911 25. 677	1.00 20.07 1.00 17.78	B B	C
ATOM	10574	CG	ARG	596	99. 233	36. 247	24. 756	1.00 17.16	В	C C
ATOM ATOM	10575 10576	CD	ARG	596	99.655	35. 296	23.636	1.00 17.14	В	C
ATOM	10570	NE CZ	ARG ARG	596 596	98. 553 98. 102	34. 982 35. 816	22. 728 21. 795	1.00 17.97 1.00 19.85	B B	N C
ATOM	10578	NH1	ARG	596	98.671	37.005	21.640	1.00 21.47	В	N
ATOM ATOM	10579 10580	NH2 C	ARG	596	97.060	35.486	21.045	1.00 18.12	В	N
ATOM	10581	0	ARG ARG	596 596	96. 692 95. 731	35. 655 35. 213	27. 632 27. 005	1.00 21.03 1.00 22.67	B B	C 0
ATOM	10582	N	ARG	597	96.811	35. 529	28. 948	1.00 20.90	В	N N
ATOM	10583	CA	ARG	597	95. 831	34.770	29.714	1.00 20.85	В	C

					F I	G.	4 -	217				(Co	ntinued)
ATOM							414	30.078	1.00	23.88	В	C	
ATOM								29.300		31.40	В	C	
ATOM								27.810		34.67	В	C	
ATOM								27.059		35.49	В	N	
ATOM ATOM				597				25. 759		35.98	В	C	
ATOM			1 ARG 2 ARG	597				25. 075		35. 20	В	N	
ATOM		C	ARG	597 597				25. 145		39.12	В	N	
ATOM			ARG	.597				30. 976 31. 945		18.83	В	C	
ATOM			LEU	598	0 1. 00			30. 964		16.66	B B	O N	
ATOM			LEU	598				32. 125		15.71	В	C	
ATOM	10595	CB	LEU	598				31. 769		12.95	В	Č	
ATOM	10596	CG	LEU	598	95.52			32. 248		12.69	В	č	
ATOM	10597		LEU	598	96.93			32.106		11.40	B	Č	
ATOM	10598		2 LEU	598	95.36		267	31.466	1.00		В	Č	
ATOM	10599	C	LEU	598	93. 36			32.642	1.00	17.19	В	C	
ATOM	10600	0	LEU	598	92. 53			31.863		17. 25	В	0	
ATOM	10601	N	GLY	599	93. 20			33. 961		16.06	В	N	
ATOM ATOM	10602 10603	CA C	GLY GLY	599 599	91.99			34. 547		16.44	В	C	
ATOM	10604	Ö	GLY	599	91. 98 90. 92			34. 735		17.37	В	C -	
ATOM	10605	N	THR	600	93. 16			34. 843 34. 786		17. 28 17. 73	В	0	
ATOM	10606	CA	THR	600	93. 24			34. 972		17. 75	B B	N C	
ATOM	10607	CB	THR	600	93. 82			33. 722		18. 93	В	Č	
ATOM	10608		THR	600	95. 18			33. 530		17.74	В	ő	
ATOM	10609		THR	600	93.000			32. 491		17.48	B	Č	
ATOM	10610	C	THR	600	94. 08			36. 183		19.93	В	Č	
ATOM	10611	0	THR	600	93. 57			37. 295		21.69	В	0	
ATOM ATOM	10612	N	PHE	601	95. 387			35. 971		21.11	В	N	
ATOM	10613 10614	CA CB	PHE PHE	601	96. 279			37. 048		21.56	В	C	
ATOM	10615	CG	PHE	601 601	97.686			36. 494		20.77	В	C	
ATOM	10616		PHE	601	97. 757 98. 676			35. 475 34. 439		21.75	В	C	
ATOM	10617	CD2	PHE	601	96. 896			35. 539		23. 50 21. 83	B B	C C	
	10618	CE1	PHE	601	98. 731			33. 474		24. 75	В	C	
ATOM	10619	CE2	PHE	601	96. 949			34. 581		22. 61	В	C	
ATOM	10620	CZ	PHE	601	97. 868			33. 547		20.03	В	Č	
ATOM	10621	C	PHE	601	96. 346			38. 244		21.61	B	Č	
ATOM	10622	0	PHE	601	96. 437			39. 386		23.03	B	Ŏ	
	10623		GLU	602	96. 312			37. 997	1.00	20.14	В	N	
ATOM	10624	CA	GLU	602	96. 374			39. 097		19.30	В	C	
ATOM	10625	CB	GLU	602	96. 505			38. 581		16.90	В	C	
ATOM ATOM	10626 10627	CG	GLU	602	95. 193			38. 135		17.16	В	C	
ATOM	10628	CD	GLU GLU	602	94. 857			86.661		17. 31	В	C	
ATOM	10629		GLU	602 602	94. 930 94. 505			86. 184		18.92	В	0	
ATOM	10630	C	GLU	602	94. 505 95. 111	37. 83 34. 83		15. 981		16.38	В	0	
ATOM	10631	Õ	GLU	602	95. 111 95. 170			19. 952 1. 179		18. 97 18. 54	B B	C 0	
ATOM	10632	N	VAL	603	93. 979	34. 5		9. 296		19. 02	В	N	
		-		500		0 10 0	٠. ١	J. 400	1.00	10.00	U	11	

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						(Continued)
					FIG. 4-218	(Continued)
			•		110.1 210	
ATOM	10633	CA	VAL	603	92. 696 34. 413 39. 984 1. 00 21. 62 B	C
ATOM	10634	CB	VAL	603	91. 513 34. 471 38. 999 1. 00 21. 51 B	C
ATOM	10635		VAL	603	90. 233 34. 055 39. 701 1. 00 19. 24 B	C
ATOM	10636		VAL	603	91. 380 35. 876 38. 442 1. 00 21. 00 B	С
ATOM	10637	Ç	VAL	603	92. 643 33. 073 40. 716 1. 00 22. 35 B	C
ATOM	10638	0	VAL	603	92. 160 32. 989 41. 848 1. 00 21. 06 B	0
ATOM	10639	N	GLU	604	93. 141 32. 031 40. 059 1. 00 22. 98 B	N
ATOM	10640	CA	GLU	604	93. 182 30. 702 40. 656 1. 00 26. 04 B	C
ATOM	10641	CB	GLU	604	93. 721 29. 681 39. 645 1. 00 28. 46 B	C
ATOM	10642	CC	GLU	604	92. 956 29. 671 38. 326 1. 00 35. 94 B	C
ATOM ATOM	10643 10644	CD OE1	GLU GLU	604	93. 559 28. 742 37. 273 1. 00 40. 17 B	C
ATOM	10645		GLU	604 604	93. 215 28. 911 36. 076 1. 00 40. 47 B 94. 360 27. 844 37. 637 1. 00 41. 61 B	0
ATOM	10646	C	GLU	604	94. 360 27. 844 37. 637 1. 00 41. 61 B 94. 072 30. 705 41. 905 1. 00 24. 63 B	C C
ATOM	10647	Ö	GLU	604	93. 657 30. 255 42. 976 1. 00 25. 47 B	0
ATOM	10648	N	ASP	605	95. 286 31. 234 41. 775 1. 00 22. 17 B	N N
ATOM	10649	CA	ASP	605	96. 213 31. 255 42. 900 1. 00 21. 12 B	C
ATOM	10650	CB	ASP	605	97. 568 31. 827 42. 463 1. 00 23. 09 B	Č
ATOM	10651	CG	ASP	605	98. 263 30. 958 41. 414 1. 00 24. 43 B	č
ATOM	10652		ASP	605	97. 894 29. 774 41. 266 1. 00 26. 59 B	ŏ
ATOM	10653		ASP	605	99. 188 31. 453 40. 742 1. 00 25. 60 B	ŏ
ATOM	10654	C	ASP	605	95. 712 31. 967 44. 159 1. 00 19. 42 B	Č
ATOM	10655	0	ASP	605	96. 099 31. 598 45. 260 1. 00 19. 67 B	0
ATOM	10656	N	GLN	606	94. 868 32. 983 44. 014 1. 00 17. 23 B	N
ATOM	10657	CA	GLN	606	94. 337 33. 673 45. 192 1. 00 16. 41 B	C
ATOM	10658	CB	GLN	606	93. 576 34. 951 44. 795 1. 00 17. 09 B	C
ATOM	10659	CG	GLN	606	94. 407 36. 070 44. 165 1. 00 15. 81 B	C
ATOM	10660	CD	GLN	606	95. 332 36. 748 45. 162 1. 00 15. 36 B	C
ATOM	10661		GLN	606	94. 879 37. 283 46. 173 1. 00 13. 19 B	0
ATOM	10662		GLN	606	96. 637 36. 730 44. 878 1. 00 14. 39 B	N
ATOM	10663	C	GLN	606	93. 360 32. 706 45. 878 1. 00 15. 71 B	C
ATOM ATOM	10664 10665	O N	GLN ILE	606	93. 337 32. 583 47. 102 1. 00 14. 30 B	0
ATOM	10666	CA	ILE	607 607	92. 549 32. 030 45. 070 1. 00 13. 95 B	N
ATOM	10667	CB	ILE	607	91. 584 31. 076 45. 583 1. 00 13. 95 B	C
ATOM	10668		ILE	607	90.772 30.437 44.448 1.00 12.90 B 89.925 29.294 44.996 1.00 11.78 B	C
ATOM	10669		ILE	607	89. 925 29. 294 44. 996 1. 00 11. 78 B 89. 909 31. 504 43. 773 1. 00 12. 90 B	C C
ATOM	10670		ILE	607	89.162 31.016 42.560 1.00 11.00 B	C
ATOM	10671	C	ILE.	607	92. 330 29. 985 46. 318 1. 00 15. 04 B	Č
ATOM	10672	Ŏ	ILE	607	92. 008 29. 670 47. 462 1. 00 15. 40 B	ŏ
ATOM	10673	Ň	GLU	608	93. 331 29. 413 45. 652 1. 00 16. 29 B	N
ATOM	10674	CA	GLU	608	94. 144 28. 359 46. 246 1. 00 18. 48 B	č
ATOM	10675	CB	GLU	608	95. 180 27. 864 45. 235 1. 00 18. 74 B	č
ATOM	10676	CG	GLU	608	96. 164 26. 851 45. 792 1. 00 22. 43 B	č
ATOM	10677	CD	GLU	608	95. 498 25. 557 46. 213 1. 00 29. 00 B	č
ATOM	10678	0E1	GLU	608	96. 096 24. 817 47. 032 1. 00 32. 52 B	Ō
ATOM	10679		GLU	608	94. 382 25. 274 45. 721 1. 00 31. 62 B	0
ATOM	10680	C	GLU	608	94. 848 28. 889 47. 501 1. 00 20. 58 B	C
ATOM	10681	0	GLU	608	95. 114 28. 138 48. 446 1. 00 23. 01 B	0

					FIG	. 4 -	219			(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	10683 10684 10685 10686 10687 10688 10699 10691 10692 10693 10694 10695 10696 10697 10698 10699 10700 10701	CA CB C O N CA CB CC CD NE CZ NHI NH2 C	ALA ALA ALA ALA ALA ALA ARG ARG ARG ARG ARG ARG ARG ARG ARG	609 609 609 610 610 610 610 611	95. 150 95. 811 96. 269 94. 826 95. 152 93. 618 92. 580 91. 317 92. 300 92. 256 92. 119 91. 838 91. 886 91. 518 91. 547 90. 501 90. 628 91. 764 89. 615	30. 183 30. 789 32. 196 30. 819 30. 426 31. 286 31. 358 31. 963 29. 952 29. 694 29. 044 27. 647 26. 826 25. 372 24. 668 25. 152 25. 223 24. 848 25. 645	47. 506 48. 646 48. 310 49. 797 50. 915 49. 516 50. 535 49. 957 51. 024 52. 223 50. 073 50. 374 49. 087 49. 260 47. 925 47. 028 45. 706 45. 129. 44. 956	1. 00 19. 99 1. 00 21. 28 1. 00 19. 81 1. 00 21. 63 1. 00 21. 88 1. 00 25. 56 1. 00 25. 56 1. 00 25. 97 1. 00 28. 12 1. 00 28. 88 1. 00 27. 27 1. 00 28. 40 1. 00 30. 54 1. 00 33. 73 1. 00 36. 39 1. 00 37. 15 1. 00 29. 24	B B B B B B B B B B B B B B B B B B B	N C C C O N C C C C N C N C N N
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	10701 10702 10703 10704 10705 10706 10707 10708 10710 10711 10712 10713 10714 10715 10716 10717 10718 10719 10720 10721 10722 10723	O N CA CB CG CD N CA CB CG CD1 CD2 CE1	ARG GLN N GLN GLN PHE HE H	611 612 612 612 612 612 612 613 613 613 613 613 613 613 613	92. 446 2 94. 092 2 95. 105 2 96. 491 2 96. 738 2 98. 183 2 99. 097 2 98. 400 2 95. 109 2 95. 441 2 94. 740 2 94. 727 3 95. 651 3 96. 974 3 95. 385 3 98. 024 3 96. 419 3 97. 742 33 97. 742 93. 531 23	2. 156 3. 432 3. 109 9. 214 9. 216	48. 848 53. 524 54. 545 53. 533 54. 784 54. 538 53. 775 54. 058 52. 796 53. 371 52. 109 52. 394 55. 607 56. 830	1.00 29.24 1.00 30.51 1.00 30.24 1.00 30.75 1.00 29.62 1.00 31.27 1.00 32.19 1.00 32.20 1.00 31.36 1.00 32.39 1.00 30.50 1.00 30.43 1.00 30.43 1.00 30.43 1.00 32.48 1.00 32.48	B B B B B B B B B B B B B B B B B B B	C O N C C C C C C C C C C C C C C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	10724 10725 10726 10727 10728 10729 10730	CA CB OG C O N	SER SER SER SER SER LYS LYS	614 614 614 614 614 615 615	91. 292 23 90. 141 23 90. 419 23 91. 609 26 90. 908 26 92. 670 26	8. 286 8. 104 7. 055 6. 953 6. 519 6. 307	55. 600 54. 607 53. 697 56. 264 57. 178 55. 797	1. 00 31. 43 1. 00 34. 43 1. 00 34. 39 1. 00 35. 74 1. 00 37. 21 1. 00 36. 52 1. 00 37. 25	B B B B B	N C C O C O N C

					FIG. 4-220	(Continued)
ATOM	10731	CB	LYS	615	93. 781 24. 196 55. 283 1. 00 37. 94 B	С
ATOM	10732	CG	LYS	615	92. 839 23. 516 54. 293 1. 00 40. 25 B	С
ATOM	10733	CD	LYS	615	93. 595 23. 050 53. 053 1. 00 42. 18 B	С
ATOM	10734	CE	LYS	615	94. 883 22. 317 53. 419 1. 00 42. 76 B	C
ATOM	10735	NZ	LYS	615	95. 776 22. 147 52. 237 1. 00 43. 07 B	N
ATOM	10736	C	LYS	615	94.001 25.231 57.544 1.00 37.98 B	C
ATOM	10737	0	LYS	615	94. 379 24. 275 58. 217 1. 00 40. 67 B	0
ATOM	10738	N	MET	616	94. 373 26. 474 57. 809 1. 00 37. 04 B	N
ATOM	10739	CA	MET	616	95. 240 26. 744 58. 948 1. 00 36. 91 B	C
ATOM	10740	CB	MET	616	96. 021 28. 047 58. 738 1. 00 36. 80 B	C
ATOM	10741	CG	MET	616	97. 042 27. 961 57. 613 1. 00 36. 28 B	C
ATOM	10742	SD	MET	616	97. 847 29. 532 57. 282 1. 00 40. 04 B	S
ATOM ATOM	10743 10744	CE	MET	616	99. 135 29. 023 56. 125 1. 00 35. 34 B	C
ATOM	10744	C 0	MET MET	616 616	94. 370 26. 817 60. 200 1. 00 35. 92 B	C
ATOM	10746	N	GLY	617	93. 181 27. 143 60. 130 1. 00 35. 52 B 94. 973 26. 514 61. 343 1. 00 33. 40 B	0
ATOM	10747	CA	GLY	617		N
ATOM	10748	C	GLY	617		C
ATOM	10749	ŏ	GLY	617	93. 584 27. 783 63. 072 1. 00 29. 42 B 92. 516 27. 729 63. 689 1. 00 30. 60 B	C
ATOM	10750	N	PHE	618	94. 202 28. 926 62. 797 1. 00 26. 74 B	O N
ATOM	10751	CA	PHE	618	93. 676 30. 204 63. 271 1. 00 25. 54 B	C
ATOM	10752	CB	PHE	618	94. 852 31.118 63. 636 1.00 26.06 B	Č
ATOM	10753	CG	PHE	618	95. 898 31. 216 62. 563 1. 00 25. 52 B	Č
ATOM	10754		PHE	618	95. 763 32. 127 61. 523 1. 00 25. 78 B	Č
ATOM	10755		PHE	618	97. 012 30. 385 62. 588 1. 00 25. 30 B	č
ATOM	10756	CE1	PHE	618	96. 726 32. 214 60. 518 1. 00 26. 10 B	č
ATOM	10757	CE2	PHE	618	97. 981 30. 459 61. 590 1. 00 26. 94 B	č
ATOM	10758	CZ	PHE	618	97. 836 31. 380 60. 549 1. 00 27. 08 B	Č
ATOM	10759	C	PHE	618	92. 706 30. 948 62. 353 1. 00 24. 88 B	Č
ATOM	10760	0	PHE	618	92. 319 32. 079 62. 644 1. 00 24. 17 B	0
ATOM	10761	N	VAL	619	92. 297 30. 313 61. 259 1. 00 24. 78 B	N
ATOM	10762	CA	VAL	619	91. 381 30. 947 60. 324 1. 00 25. 04 B	C
ATOM	10763	CB	VAL	619	91. 913 30. 876 58. 875 1. 00 25. 17 B	С
ATOM	10764		VAL	619	91. 007 31. 665 57. 945 1. 00 23. 09 B	C
ATOM ATOM	10765		VAL	619	93. 326 31. 415 58. 817 1. 00 26. 33 B	C
ATOM	10766 10767	C	VAL	619	90. 004 30. 303 60. 371 1. 00 25. 53 B	C
ATOM	10768	O N	VAL ASP	619	89. 873 29. 083 60. 378 1. 00 25. 84 B	0
ATOM	10769	CA	ASP	620	88. 981 31. 146 60. 405 1. 00 26. 00 B	N
ATOM	10770	CB	ASP	620 620	87.601 30.701 60.449 1.00 26.41 B 86.779 31.717 61.238 1.00 26.64 B	C
ATOM	10771	CG	ASP	620	07.004	C .
ATOM	10772		ASP	620	04 504 05 05 05	C
ATOM	10773		ASP	620	01 044 00	0
ATOM	10774	C	ASP	620	84. 914 30. 306 60. 765 1. 00 26. 86 B 87. 104 30. 610 59. 011 1. 00 27. 59 B	0 C
ATOM	10775	ŏ	ASP	620	86. 687 31. 610 58. 435 1. 00 27. 47 B	0 .
ATOM	10776	Ň	ASN	621	87. 144 29. 409 58. 438 1. 00 29. 06 B	N N
ATOM	10777	CA	ASN	621	86. 733 29. 213 57. 053 1. 00 30. 04 B	C
ATOM	10778	CB	ASN	621	86. 925 27. 752 56. 622 1. 00 33. 33 B	C
ATOM	10779	CG	ASN	621	86. 022 26. 782 57. 377 1. 00 36. 94 B	č
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	FIG. 4-221	(Continued)
ATOM 10780 OD1 ASN 621 ATOM 10781 ND2 ASN 621 ATOM 10782 C ASN 621 ATOM 10783 O ASN 621 ATOM 10784 N LYS 622 ATOM 10785 CA LYS 622 ATOM 10786 CB LYS 622 ATOM 10787 CG LYS 622 ATOM 10788 CD LYS 622 ATOM 10789 CE LYS 622 ATOM 10790 NZ LYS 622 ATOM 10790 NZ LYS 622 ATOM 10791 C LYS 622 ATOM 10792 O LYS 622 ATOM 10793 N ARG 623 ATOM 10794 CA ARG 623 ATOM 10795 CB ARG 623 ATOM 10796 CG ARG 623 ATOM 10797 CD ARG 623 ATOM 10798 NE ARG 623 ATOM 10798 NE ARG 623 ATOM 10799 CZ ARG 623 ATOM 10800 NH1 ARG 623 ATOM 10801 NH2 ARG 623 ATOM 10801 NH2 ARG 623 ATOM 10802 C ARG 623 ATOM 10804 N ILE 624 ATOM 10805 CA ILE 624 ATOM 10807 CG2 ILE 624 ATOM 10807 CG2 ILE 624 ATOM 10807 CG2 ILE 624 ATOM 10808 CG1 ILE 624	84. 795 26. 940 57. 415 1. 00 38. 23 86. 630 25. 763 57. 972 1. 00 39. 37 85. 310 29. 639 56. 756 1. 00 29. 63 84. 887 29. 626 55. 604 1. 00 30. 93 84. 563 30. 007 57. 787 1. 00 28. 32 83. 195 30. 441 57. 573 1. 00 27. 00 82. 303 29. 986 58. 740 1. 00 29. 24 82. 062 28. 471 58. 738 1. 00 32. 47 81. 029 28. 002 59. 761 1. 00 33. 84 81. 571 29. 501 61. 703 1. 00 36. 73 83. 168 31. 957 57. 404 1. 00 25. 42 82. 145 32. 543 57. 047 1. 00 26. 19 84. 314 32. 583 57. 642 1. 00 21. 83 84. 436 34. 023 57. 515 1. 00 18. 89 84. 380 34. 664 58. 895 1. 00 17. 53 83. 122 34. 394 60. 991 1. 00 19. 29 83. 405 35. 632 61. 690 1. 00 19. 11 84. 207 35. 718 <	B O B O N B C C B B C C B B C C B B B C C B B B C C B B B B B B B B B B B B B B B B B B B B
ATOM 10805 CA ILE 624 ATOM 10806 CB ILE 624 ATOM 10807 CG2 ILE 624 ATOM 10808 CG1 ILE 624 ATOM 10809 CD1 ILE 624 ATOM 10810 C ILE 624 ATOM 10811 O ILE 624 ATOM 10812 N ALA 625 ATOM 10813 CA ALA 625 ATOM 10814 CB ALA 625 ATOM 10815 C ALA 625 ATOM 10816 O ALA 625 ATOM 10817 N ILE 626 ATOM 10818 CA ILE 626 ATOM 10819 CB ILE 626 ATOM 10820 CG2 ILE 626 ATOM 10821 CG1 ILE 626 ATOM 10822 CD1 ILE 626 ATOM 10823 C ILE 626	86. 769 34. 798 54. 629 1. 00 16. 59 87. 439 33. 572 53. 991 1. 00 18. 45 88. 563 34. 017 53. 059 1. 00 18. 66 87. 971 32. 647 55. 088 1. 00 19. 91 88. 623 31. 385 54. 564 1. 00 22. 12 86. 230 35. 695 53. 519 1. 00 16. 74 85. 402 35. 268 52. 710 1. 00 17. 92 86. 688 36. 939 53. 494 1. 00 15. 59 85. 816 39. 174 53. 155 1. 00 18. 31 87. 375 38. 159 51. 503 1. 00 16. 49 87. 149 39. 107 50. 598 1. 00 16. 75 88. 158 39. 454 49. 608 1. 00 17. 73 88. 207 38. 397 48. 478 1. 00 19. 21 86. 883 38. 365 47. 742 1. 00 19. 01 89. 348 38. 713 47. 511 1. 00 18. 94 89. 576 37. 642 46. 471 1. 00 20. 78	B C B C B C B C B C B C B C B C B C B C
ATOM 10824 O ILE 626 ATOM 10825 N TRP 627 ATOM 10826 CA TRP 627 ATOM 10827 CB TRP 627 ATOM 10828 CG TRP 627	87. 850 40. 810 49. 003 1. 00 17. 46 86. 692 41. 116 48. 754 1. 00 18. 15 88. 878 41. 628 48. 781 1. 00 16. 65 88. 663 42. 938 48. 177 1. 00 15. 95 88. 215 43. 945 49. 231 1. 00 14. 07 89. 318 44. 713 49. 875 1. 00 12. 00	B C B C B C B C

	·						0.00			(Continued)
					FIC	3.4-	222			
ATOM	10829	CD2		627	89.641	46.084	49.646	1.00 11.41	В	C
ATOM	10830		TRP	627	90.725	46.410	50.500	1.00 10.99	В	C
ATOM	10831	CE3		627	89. 121	47.074	48.806	1.00 9.75	В	C
ATOM	10832	CD1	TRP	627	90. 198	44.267	50.826	1.00 14.55	В	С
ATOM	10833	NE1	TRP	627	91.046	45. 283	51.208	1.00 10.25	В	N
ATOM	10834	CZ2	TRP	627	91.289	47.681	50.536	1.00 9.06	В	С
ATOM	10835	CZ3	TRP	627	89.685	48.340	48.844	1.00 9.47	В	С
ATOM	10836	CH2	TRP	627	90.755	48.632	49.702	1.00 8.43	В	С
ATOM	10837	C	TRP	627	89.881	43. 489	47. 433	1.00 17.27	В	С
ATOM	10838	0	TRP	627	91.027	43. 146	47.732	1.00 16.96	В	0
ATOM	10839	N	GLY	628	89.613	44. 351	46.459	1.00 16.52	В	N
ATOM	10840	CA	GLY	628	90.672	44.947	45.675	1.00 16.52	В	С
ATOM	10841	C	GLY	628	90.186	46. 198	44.975	1.00 17.44	В	C
ATOM	10842	0	GLY	628	88.977	46.441	44.887	1.00 17.88	В	0
ATOM	10843	N	TRP	629	91.132	46.989	44.479	1.00 15.93	В	N
ATOM	10844	CA	TRP	629	90.841	48.235	43. 781	1.00 15.93	В	C
ATOM	10845	CB	TRP	629	91.480	49.395	44.552	1.00 13.57	В	C
MOTA	10846	CG	TRP	629	90.867	50.763	44.341	1.00 14.96	В	С
ATOM	10847	· CD2	TRP	629	90.389	51.656	45.360	1.00 13.15	В	С
ATOM	10848	CE2	TRP	629	89.944	52.830	44.712	1.00 13.17	В	C .
ATOM	10849	CE3		629	90.296	51.577	46.758	1.00 14.07	В	C
ATOM	10850	CD1	TRP	629	90.694	51.419	43. 149	1.00 14.45	В	С
ATOM	10851	NE1	TRP	629	90. 141	52.657	43.366	1.00 12.77	В	N
ATOM	10852	CZ2		629	89.411	53. 921	45.414	1.00 13.59	В	С
ATOM	10853	CZ3	TRP	629	89.767	52.660	47.461	1.00 14.81	В	С
ATOM	10854	CH2	TRP	629	89.330	53.820	46. 782	1.00 15.16	В	C
ATOM	10855	C	TRP	629	91.481	48.074	42.399	1.00 17.34	В	C
ATOM	10856	0	TRP	629	92.571	47.517	42. 285	1.00 18.55	В	0
ATOM	10857	N	SER	630	90.802	48. 538	41.354	1.00 17.70	В	N
ATOM	10858	CA	SER	630	91.309	48. 430	39. 982	1.00 17.70	В	С
ATOM	10859	CB	SER	630	92.649	49. 144	39.846	1.00 18.19	В	C
ATOM	10860	0G	SER	630	92.574	50. 437	40.404	1.00 24.67	В	0
ATOM	10861	C	SER	630	91.477	46.977	39. 563	1.00 17.40	В	C
ATOM	10862	0	SER	630	90. 501	46. 235	39.469	1.00 18.69	В	0
ATOM	10863	N	TYR	631	92.712	46. 565	39. 304	1.00 16.34	В	Ŋ
ATOM	10864	CA	TYR	631	92. 951	45. 192	38. 904	1.00 15.96	В	C
ATOM	10865	CB	TYR	631	94.430	44. 973	38. 579	1.00 15.36	В	C
ATOM	10866	CG	TYR	631	94.689	43. 709	37. 779	1.00 15.93	В	Č
ATOM	10867	CD1	TYR	631	94.626	42. 450	38. 380	1.00 15.38	В	C
ATOM	10868	CE1	TYR	631	94.830	41. 287	37. 634	1.00 16.25	В	C
ATOM	10869		TYR	631	94. 961	43. 773	36. 409	1.00 15.67	В	C
ATOM	10870			631	95.160	42.620	35.655	1.00 13.59	В	C
ATOM	10871	CZ	TYR	631	95.092	41.384	36. 270	1.00 15.96	В	C
ATOM	10872	OH	TYR	631	95. 264	40. 243	35. 525	1.00 14.59	В	0
ATOM	10873	C	TYR	631	92.499	44. 286	40.049	1.00 15.68	В	C
ATOM	10874	0	TYR	631	91.949	43. 213	39. 824	1.00 16.42	В	0
ATOM	10875	N	GLY	632	92. 723	44. 729	41. 281	1.00 15.56	В	N
ATOM	10876	CA	GLY	632	92. 292	43. 950	42. 429	1.00 14.43	В	C
ATOM	10877	C	GLY	632	90.777	43.807	42. 398	1.00 13.07	В	С

					FIG. 4-223	(Cor	ntinued)
ATOM	10070	0	CI V	gaa		•	
ATOM	10878 10879	O N	GLY GLY	$\begin{array}{c} 632 \\ 633 \end{array}$	90. 239 42. 771 42. 777 1. 00 12. 09 B 90. 087 44. 855 41. 946 1. 00 12. 57 B	0	
ATOM	10880	CA	GLY	633	90. 087 44. 855 41. 946 1. 00 12. 57 B 88. 637 44. 800 41. 846 1. 00 10. 88 B	N C	
ATOM	10881	C	GLY	633	88. 271 43. 743 40. 818 1. 00 10. 78 B	C	
ATOM	10882	Ŏ	GLY	633	87. 337 42. 956 40. 986 1. 00 9. 26 B	ŏ	
ATOM	10883	N	TYR	634	89. 031 43. 729 39. 734 1. 00 11. 33 B	N	
ATOM	10884	CA	TYR	634	88. 822 42. 755 38. 682 1. 00 11. 09 B	Č	
ATOM	10885	CB	TYR	634	89. 860 42. 951 37. 595 1. 00 7. 35 B	č	
ATOM	10886	CG	TYR	634	89.815 41.899 36.526 1.00 8.04 B	Č	
ATOM	10887		TYR	634	90.949 41.162 36.204 1.00 7.58 B	C	
ATOM	10888	CE 1		634	90.924 40.218 35.189 1.00 7.56 B	C	
ATOM	10889		TYR	634	88.649 41.660 35.805 1.00 8.82 B	C	
ATOM	10890		TYR	634	88. 615 40. 715 34. 788 1. 00 7. 88 B	C	•
ATOM	10891	CZ	TYR	634	89. 756 39. 996 34. 488 1. 00 6. 90 B	C	
ATOM	10892	OH	TYR	634	89. 722 39. 039 33. 504 1. 00 8. 03 B	0	
ATOM ATOM	10893 10894	C	TYR	634	88. 967 41. 358 39. 278 1. 00 13. 02 B	C	
ATOM	10895	O N	TYR VAL	634 635	88. 038 40. 548 39. 222 1. 00 13. 14 B	0	
ATOM	10896	CA	VAL	635	90.140 41.091 39.858 1.00 14.38 B 90.426 39.796 40.467 1.00 13.39 B	N	
ATOM	10897	CB	VAL	635		C	
ATOM	10898		VAL	635	91. 839 39. 747 41. 093 1. 00 13. 28 B 91. 995 38. 467 41. 923 1. 00 13. 06 B	C	
ATOM	10899		VAL	635	92. 894 39. 782 39. 999 1. 00 8. 09 B	C C	
ATOM	10900	C	VAL	635	89. 412 39. 443 41. 533 1. 00 13. 35 B	C	
ATOM	10901	0	VAL	635	88. 932 38. 320 41. 563 1. 00 15. 02 B	Õ	
ATOM	10902	N	THR	636	89. 091 40. 394 42. 405 1. 00 13. 48 B	Ň	
ATOM	10903	CA	THR	636	88. 108 40. 160 43. 457 1. 00 13. 74 B	Ċ	
ATOM	10904	CB	THR	636	87. 788 41. 451 44. 260 1. 00 15. 19 B	Č	
ATOM	10905	0G1		636	88. 950 41. 886 44. 978 1. 00 15. 24 B	0	
ATOM	10906		THR	636	86. 655 41. 188 45. 259 1. 00 13. 51 B	C	
ATOM	10907	C	THR	636	86. 792 39. 665 42. 862 1. 00 14. 57 B	C	
ATOM	10908	0	THR	636	86. 160 38. 750 43. 395 1. 00 15. 29 B	0	
ATOM ATOM	10909	N	SER	637	86. 373 40. 281 41. 762 1. 00 15. 59 B	N	
ATOM	10910 10911	CA CB	SER SER	637	85. 120 39. 905 41. 112 1. 00 15. 99 B	C	
ATOM	10912	OG	SER	637 637	84. 698 40. 974 40. 102 1. 00 16. 88 B 84. 303 42. 158 40. 766 1. 00 18. 07 B	C	
ATOM	10913	C	SER	637	0	0	
ATOM	10914	ŏ	SER	637		C	
ATOM	10915	Ň	MET	638	84. 250 37. 773 40. 487 1. 00 17. 87 B 86. 309 38. 300 39. 740 1. 00 15. 64 B	0 N	
ATOM	10916	ĊA	MET	638	86. 493 37. 030 39. 052 1. 00 15. 55 B	N C	
ATOM	10917	CB	MET	638	87. 807 37. 033 38. 272 1. 00 15. 97 B	C	
ATOM	10918	ĆG	MET	638	87. 822 37. 959 37. 067 1. 00 17. 38 B	C	
ATOM	10919	SD	MET	638	86. 715 37. 422 35. 736 1. 00 19. 14 B	Š	
ATOM	10920	CE	MET	638	87. 806 36. 324 34. 798 1. 00 15. 28 B	Č	
ATOM	10921	C	MET	638	86. 511 35. 913 40. 093 1. 00 17. 56 B	č	
ATOM	10922		MET	638	86. 018 34. 807 39. 843 1. 00 17. 45 B	Ŏ	
ATOM	10923	N	VAL	639	87. 086 36. 199 41. 260 1. 00 16. 50 B	N	
ATOM	10924	CA	VAL	639	87. 133 35. 207 42. 317 1. 00 17. 27 B	C	
ATOM	10925	CB	VAL	639	88. 047 35. 640 43. 480 1. 00 16. 78 B	C	
ATOM	10926	CG1	VAL	639	87. 648 34. 884 44. 757 1. 00 16. 23 B	С	

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											(Continued	1/
						FIC	3. 4 -	224			Continued	1)
•						*						
	ATOM	10927		VAL	639	89.495	35. 335	43. 139	1.00 14.45	В	C	
	ATOM	10928	C	VAL	639	85.742	34. 919	42.875	1.00 17.57	В	C	
	ATOM	10929	0	VAL	639	85. 387	33.760	43.081	1.00 18.52	В	0	
	ATOM	10930	N	LEU	640	84. 957	35.964	43. 124	1.00 16.90	В	N	
	ATOM	10931	CA	LEU	640	83.618	35. 766	43.661	1.00 17.42	В	C	
	ATOM	10932	CB	LEU	640	82.978	37.098	44. 032	1.00 17.45	В	C	
	ATOM	10933	CG	LEU	640	83. 512	37.699	45. 327	1.00 17.52	В	C C	
	ATOM	10934		LEU	640	82. 743	38. 962	45.654	1.00 14.30	В	C	
	ATOM	10935		LEU	640	83.378	36.677	46.447	1.00 15.97	В	C C	
	ATOM	10936	C	LEU	640	82. 713	35. 020	42.699	1.00 17.81	В		
	ATOM	10937	0	LEU	640	81.821	34. 284	43.119	1.00 20.73	В	0	
	ATOM	10938	N	GLY	641	82.952	35. 198	41.409	1.00 18.14	В	N	
	ATOM ATOM	10939	CA	GLY	641	82.135	34. 526	40.418	1.00 17.61	В	C	
	ATOM	10940 10941	C	GLY GLY	641 641	82.758	33. 235	39.936	1.00 17.52 1.00 15.15	B B	C 0	
	ATOM	10941	O N	SER	642	82. 346 83. 735	32. 697 32. 727	38. 911 40. 683	1.00 15.15	В	N N	
	ATOM	10942	CA	SER	642	84. 419	31.497	40. 297	1.00 17.33	В	C	
	ATOM	10944	CB	SER	642	85.841	31.479	40. 864	1.00 19.38	В	C	
	ATOM	10945	OG	SER	642	85.849	31.088	42. 226	1.00 20.16	В	0	
	ATOM	10946	Č	SER	642	83.691	30. 239	40. 755	1.00 21.75	В	Č	
	ATOM	10947	ŏ	SER	642	83. 974	29.147	40. 265	1.00 22.65	В	Ö	
	ATOM	10948	Ň	GLY	643	82.768	30. 395	41.701	1.00 22.05	B	Ň	
	ATOM	10949	CA	GLY	643	82.023	29. 258	42. 210	1.00 22.58	B	Ċ	
	ATOM	10950	C	GLY	643	82.811	28.335	43.130	1.00 24.03	В	Ċ	
	ATOM	10951	0	GLY	643	82.460	27.162	43. 271	1.00 26.05	В	0	
	ATOM	10952	N	SER	644	83.859	28.849	43.772	1.00 22.41	В	N	
	ATOM	10953	CA	SER	644	84.684	28.024	44.656	1.00 21.56	В	C	
	ATOM	10954	CB	SER	644	86.065	28.657	44.833	1.00 21.02	В	C	
	ATOM	10955	0G	SER	644	85. 992	29. 798	45.666	1.00 22.35	В	0	
	ATOM	10956	C	SER	644	84.084	27. 773	46.037	1.00 21.06	В	C	
	ATOM	10957	0	SER	644	84. 451	26.807	46. 707	1.00 23.51	В	0	
	ATOM	10958	N	GLY	645	83. 175	28.643	46. 469	1.00 19.50	В	N	
	ATOM	10959	CA	GLY	645	82. 561	28. 485	47. 774	1.00 16.85	В	C	
	ATOM	10960	C	GLY	645	83.484	28.868	48. 920	1.00 18.76	В	C	
	ATOM ATOM	10961 10962	0 N	GLY VAL	645	83.111	28. 771	50.090	1.00 18.32	В	0	
	ATOM	10962	N CA	VAL	646 646	84. 691 85. 669	29. 320 29. 695	48. 591	1.00 18.97 1.00 18.18	В	N	
	ATOM	10964	CB	VAL	646	87. 095	29. 718	49. 612 49. 029	1.00 18.18	В	C	
	ATOM	10965	CG1	VAL	646	88. 082	30. 202	50.086	1.00 19.50	B B	C C	
	ATOM	10966		VAL	646	87. 471	28. 341	48. 516	1.00 17.45	В	C	
	ATOM	10967	C	VAL	646	85. 433	31.051	50. 266	1.00 11.23	В	C	
	ATOM	10968	ŏ	VAL	646	85. 860	31. 270	51.396	1.00 18.24	В	0	
	ATOM	10969	Ň	PHE	647	84. 763	31.957	49. 561	1.00 20.76	В	N N	
	ATOM	10970	CA	PHE	647	84. 525	33. 297	50.082	1.00 16.60	В	C	
	ATOM	10971	CB	PHE	647	85.066	34. 337	49.094	1.00 16.00	В	Č	
	ATOM	10972		PHE	647	86. 528	34. 204	48. 820	1.00 15.63	В	Č	
	ATOM	10973		PHE	647	87. 455	34. 941	49. 553	1.00 14.72	B	Č	
	ATOM	10974		PHE	647	86. 985	33. 320	47. 844	1.00 14.49	. B	č	
	ATOM	10975		PHE	647	88. 826	34.800	49. 317	1.00 16.66	B	č	

	F I G. 4 - 225 (Continued)											
					ric	J. 4 ⁻	223	٠				
ATOM			2 PHE	647	88.356	33. 170	47.600	1.00 16.73	В	C		
ATOM ATOM				647	89. 278	33. 913	48. 338	1.00 13.35	В	C		
ATOM			PHE PHE	647 647	83.068	33. 604 33. 328	50.365	1.00 16.77	В	C		
ATOM			LYS	648	82. 194 82. 819	34. 214	49. 551 51. 515	1.00 17.32 1.00 16.74	В	0 N		
ATOM		CA		648	81.466	34. 565	51.905	1.00 10.74	B B	N C		
ATOM			LYS	648	81.369	34. 634	53. 429	1.00 19.04	В	C		
ATOM				648	80.069	35. 233	53.911	1.00 13.04	В	Č		
ATOM		CD		648	79.876	35.060	55.393	1.00 23.19	B	č		
ATOM		CE	LYS	648	78. 548	35.645	55.814	1.00 24.97	B	Č		
ATOM		NZ	LYS	648	78. 180	35. 150	57.165	1.00 31.55	В	N		
ATOM	10987	C	LYS	648	81.019	35. 900	51.308	1.00 21.05	В	C		
ATOM	10988	0	LYS	648	79.851	36.070	50. 930	1.00 20.25	В	0		
ATOM ATOM	10989 10990	N CA	CYS CYS	649	81.954	36. 842	51. 237	1.00 20.69	В	N		
ATOM	10991	CA	CYS	$649 \\ 649$	81. 670 82. 928	38. 163	50. 711	1.00 21.97	В	C		
ATOM	10992	0	CYS	649	84. 054	38. 811 38. 437	50. 134 50. 477	1.00 22.72 1.00 23.68	В	C		
ATOM	10993	ČB	CYS	649	81.124	39. 045	51.822	1.00 23.08	B B	0 C		
ATOM	10994	SG	CYS	649	82. 287	39. 215	53. 208	1.00 26.89	В	S		
ATOM	10995	N	GLY	650	82. 728	39. 796	49. 267	1.00 20.11	В	N .		
ATOM	10996	CA	GLY	650	83.850	40.476	48.668	1.00 18.42	B	Ċ		
ATOM	10997	C	GLY	650	83. 484	41.895	48.308	1.00 18.08	В	Ċ		
ATOM	10998	0	GLY	650	82. 308	42. 198	48. 135	1.00 18.19	В	0		
ATOM	10999	N	ILE	651	84. 490	42.764	48. 209	1.00 17.42	В	N		
ATOM ATOM	11000 11001	CA CB	ILE	651	84. 284	44. 162	47. 851	1.00 15.98	В	Č		
ATOM	11001		ILE ILE	651 651	84. 632	45.117	49.014	1.00 15.40	В	C		
ATOM	11002		ILE	651	84. 386 83. 789	46. 559 44. 786	48. 589	1.00 15.87	В	C		
ATOM	11004		ILE	651	84.017	45. 721	50. 242 51. 411	1.00 15.95 1.00 14.84	В	C		
ATOM	11005	C	ILE	651	85. 190	44. 512	46. 679	1.00 14.64	B B	C C		
ATOM	11006	0	ILE	651	86. 404	44. 330	46. 754	1.00 16.63	В	0		
ATOM	11007	N	ALA	652	84. 594	45.025	45.608	1.00 16.04	В	N		
ATOM	11008	CA	ALA	652		45.409	44.413	1.00 15.10	B	Č		
ATOM	11009	CB	ALA	652	84. 809	44.629	43. 214	1.00 16.38	В.	Č		
ATOM	11010	C	ALA	652		46.908	44. 153	1.00 15.88	В	C		
ATOM ATOM	11011	0	ALA	652		47. 399	43. 895	1.00 14.37	В	0		
ATOM	11012 11013	N CA	VAL	653		47. 630	44, 214	1.00 15.73	В	Ŋ		
ATOM	11013	CB	VAL VAL	653 653		49.070	43. 978	1.00 15.50	В	C		
ATOM	11015		VAL	653		49. 831 51. 327	45. 055 44. 787	1.00 17.97	В	C		
ATOM	11016		VAL	653		49. 525	46. 446	1.00 18.06 1.00 18.80	В	C .		
ATOM	11017	C	VAL	653		49. 398	42.624	1.00 15.00	B B	C		
ATOM	11018	Ŏ	VAL	653		49. 087	42. 373	1.00 13.11	В	C 0		
ATOM	11019	N	ALA	654		50. 031	41.766	1.00 14.41	В	N N		
ATOM	11020	CA	ALA	654		50. 438	40. 427	1.00 12.10	В	Č		
ATOM	11021	CB	ALA	654	87. 424	51.655	40.518	1.00 12.15	B	č		
ATOM	11022	Ç	ALA	654		49. 318	39.700	1.00 12.48	В	Č		
ATOM	11023	0	ALA	654		49. 500	39. 192	1.00 13.17	В	0		
ATOM	11024	N	PRO	655	86. 633	48. 141	39.626	1.00 11.84	В	N		

, ··•					FI	G. 4-	2 2 6	•		(Continued)
ATOM	11025	CD	PRO	655	85. 273	47. 797	40. 088	1.00 11.50	В	С
ATOM	11026	CA	PR0	655	87. 247	47.003	38.954	1.00 11.05	В	C
ATOM	11027	CB	PRO	655	86.399		39. 436	1.00 11.09	B	Č
ATOM	11028	CG	PRO	655	85.030		39. 428	1.00 8.50	B	č
ATOM	11029	Č	PRO	655	87. 190		37. 447	1.00 10.92	В	č
ATOM	11023	ŏ	PRO	655	86. 383	47.847	36. 896	1.00 10.32	B	ŏ
ATOM	11030	Ň	VAL	656	88.066	46. 352	36. 791	1.00 11.41	В	N
ATOM	11031	CA	VAL	656	88. 052	46. 250	35. 345	1.00 9.08	В	C
ATOM	11032	CB	VAL	656	89. 452	45. 888	34. 790	1.00 9.00	В	C
					89. 336					
ATOM	11034		VAL	656		45. 163	33. 451	1.00 5.90	В	C
ATOM	11035		VAL	656	90. 249		34. 601	1.00 7.63	В	C
ATOM	11036	C	VAL	656	87.107	45.056	35. 224	1.00 10.20	В	C
ATOM	11037	0	VAL	656	87. 157	44. 152	36.058	1.00 10.59	В	0
ATOM	11038	N	SER	657	86. 231	45.038	34. 230	1.00 11.76	В	N
ATOM	11039	CA	SER	657	85.313	43.908	34. 115	1.00 14.03	В	C
ATOM	11040	CB	SER	657	83.867	44.375	34. 271	1.00 13.85	В	C
ATOM	11041	0G	SER	657	83. 495	45. 242	33. 218	1.00 15.07	В	0
ATOM	11042	C	SER	657	85.456	43. 153	32.812	1.00 14.66	В	С
ATOM	11043	0	SER	657	85. 191	41.952	32. 743	1.00 17.18	В	0
ATOM	11044	N	ARG	658	85. 887	43.860	31. 781	1.00 14.15	В	N
ATOM	11045	CA	ARG	658	86.050	43.277	30.459	1.00 13.24	В	C
ATOM	11046	CB	ARG	658	84. 768	43.532	29.670	1.00 14.22	В	С
ATOM	11047	CG	ARG	658	84. 763	43.086	28. 231	1.00 18.57	В	C
ATOM	11048	CD	ARG	658	83.436	43.470	27. 588	1.00 19.40	В	C
ATOM	11049	NE	ARG	658	83.475	43. 338	26. 138	1.00 23.11	В	N ·
ATOM	11050	CZ	ARG	658	82.868	42.376	25.454	1.00 22.54	В	C
ATOM	11051	NH1	ARG	658	82.167	41.445	26.088	1.00 21.95	В	N
ATOM	11052	NH2	ARG	658	82.955	42.361	24. 131	1.00 22.77	В	N
ATOM	11053	C	ARG	658	87. 242	44.014	29.857	1.00 12.76	В	C
ATOM	11054	0	ARG	658	87. 218	45.239	29.733	1.00 11.97	В	0
ATOM	11055	N	TRP	659	88. 282	43.283	29.476	1.00 11.05	В	N
ATOM	11056	CA	TRP	659	89.468	43.942	28.955	1.00 12.23	В	C
ATOM	11057	CB	TRP	659	90.578	42.918	28.777	1.00 11.99	В	Ċ
ATOM	11058	CG	TRP	659	91.026	42.392		1.00 13.26	В	C
ATOM	11059	CD2	TRP	659	91.729	43.120	31.122	1.00 12.61	В	Č
ATOM	11060		TRP	659	91.848	42.271	32. 242	1.00 13.22	B	Č
ATOM	11061	CE3	TRP	659	92.268	44.412	31.193	1.00 14.19	В	Č
ATOM	11062		TRP	659	90.759	41.163	30.644	1.00 13.17	B	č
ATOM	11063		TRP	659	91.247	41.083	31.920	1.00 13.29	В	Ň
ATOM	11064		TRP	659	92.489	42.670	33. 424	1.00 13.99	B	ë
ATOM	11065		TRP	659	92.909	44. 810	32. 373	1.00 13.35	B	č
ATOM	11066		TRP	659	93.011	43. 940	33. 468	1.00 11.92	B	č
ATOM	11067	C	TRP	659	89. 338	44. 840	27. 730	1.00 13.23	В	č
ATOM	11068	ŏ	TRP	659	90.118	45. 766	27. 569	1.00 15.25	В	0
ATOM	11069	Ň	GLU	660	88. 361	44. 595	26. 871	1.00 13.59	В	N N
ATOM	11070	ĊA	GLU	660	88. 181	45. 453	25. 708	1.00 14.33	В	C
ATOM	11071	CB	GLU	660	87. 147	44. 854	24. 743	1.00 13.33	В	C
ATOM	11072	CG	GLU	660	87. 572	43. 527	24. 143	1.00 16.10		
ATOM	11072	CD	GLU	660					В	C
VION	11019	עט	aru	UUU	86. 452	42.829	23. 386	1.00 25.49	В	С

					FIC	3. 4	- 227			(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	11075 11076 11077 11078 11079	OE CC	TYR TYR 1 TYR 1 TYR 2 TYR 2 TYR TYR	660 660 660 661 661 661 661 661 661 662 662 662 662	86. 087 85. 929 87. 719 87. 661 87. 371 86. 941 85. 988 84. 599 83. 823 82. 553 84. 061 82. 782 82. 035 80. 785 88. 146 88. 083 89. 239 90. 411 91. 225 92. 049 93. 379 94. 168 91. 522 92. 297 93. 620 94. 395 91. 309 91. 095 92. 310 93. 192 93. 961 95. 093 95. 223 95. 869	43. 278 41. 825 46. 833 47. 769 46. 960 48. 258 48. 119 47. 597 47. 053 46. 548 47. 629 47. 123 46. 581 46. 046 49. 045 50. 266 48. 355 49. 060 48. 182 49. 021 48. 699 49. 531 50. 194 51. 030 50. 699 51. 549 49. 615 49. 337 50. 405 52. 192 51. 741 52. 327 50. 836	23. 914 26. 170 25. 375 27. 450 27. 977 29. 168 28. 872 29. 898 29. 653 27. 581 27. 323 28. 367 28. 142 28. 464 28. 555 28. 789 29. 289 30. 240 31. 187 31. 468 32. 255 31. 734 32. 520 32. 776 33. 532 28. 182 26. 996 27. 588 28. 288 29. 152 30. 243 28. 780	1. 00 29. 78 1. 00 26. 73 1. 00 14. 88 1. 00 14. 50 1. 00 14. 66 1. 00 15. 13 1. 00 15. 73 1. 00 19. 12 1. 00 18. 37 1. 00 19. 84 1. 00 19. 07 1. 00 20. 28 1. 00 20. 80 1. 00 20. 60 1. 00 14. 96 1. 00 14. 55 1. 00 14. 55 1. 00 14. 52 1. 00 13. 98 1. 00 13. 98 1. 00 13. 69 1. 00 13. 69 1. 00 13. 69 1. 00 15. 44 1. 00 15. 44 1. 00 15. 66 1. 00 13. 58 1. 00 13. 58 1. 00 13. 58 1. 00 13. 58 1. 00 13. 58 1. 00 13. 70 1. 00 13. 70 1. 00 13. 70 1. 00 13. 70 1. 00 13. 70 1. 00 13. 70 1. 00 13. 70	B B B B B B B B B B B B B B B B B B B	
ATOM ATOM	11109 11110	O N	ASP ASP SER	663 664	94. 565	50. 076 49. 045 50. 444	26. 850 27. 378 25. 612	1. 00 13. 21 1. 00 13. 05 1. 00 13. 86	B B R	C 0
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	11111 11112 11113 11114 11115 11116 11117 11118 11119 11120 11121 11122	CA CB OG C O N CA CB CG1 CG2 C	SER SER SER SER VAL VAL VAL	664 664 664 664 665 665 665 665 665	95. 321 95. 464 96. 055 96. 714 97. 066 97. 503 98. 865 99. 547 101. 023 99. 354 99. 020	49. 658 50. 364 51. 642 49. 340 48. 176 50. 371 50. 158 51. 496 51. 263 62. 519 49. 169	24. 738 23. 394 23. 550 25. 278 25. 438 25. 559 26. 041 26. 427 26. 663 25. 327 27. 206	1. 00 13. 86 1. 00 13. 65 1. 00 14. 44 1. 00 16. 79 1. 00 13. 42 1. 00 12. 83 1. 00 12. 98 1. 00 15. 86 1. 00 14. 66 1. 00 15. 28 1. 00 15. 28 1. 00 15. 25 1. 00 15. 22	B B B B B B B B	N C C O C O N C C C C C C

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									(Comtinue 1)
				FI	G. 4-	228			(Continued)
<u>ለጥብ</u>	11100		VD eee				1 00 17 07	n	N
ATOM	11123		YR 666			28. 154	1.00 17.07	В	N C
ATOM	11124		YR 666			29. 299	1.00 15.32	В	C
ATOM	11125		YR 666			30. 531	1.00 13.28	В	C
ATOM	11126		YR 666			31. 751	1.00 12.79	В	C
ATOM	11127	CD1 T				31.845	1.00 12.27	В	C
ATOM	11128	CE1 T				32.964	1.00 12.60	В	C
ATOM	11129	CD2 T				32. 809	1.00 12.83	В	C
ATOM	11130	CE2 T				33. 928	1.00 11.79	В	C
ATOM	11131		YR 666			34.005	1.00 13.90	В	C
ATOM	11132		YR 666			35. 131	1.00 12.51	В	0
ATOM	11133		YR 666			29. 023	1.00 15.26	В	C
ATOM	11134		YR 666			29.399	1.00 18.30	В	0
ATOM	11135		HR 667			28. 365	1.00 14.70	В	N
ATOM	11136 11137		HR 667			28. 097	1.00 13.70	В	C
ATOM			HR 667			27.656	1.00 12.07	В	C
ATOM ATOM	11138 11139		HR 667			28. 635	1.00 11.17	В	0
ATOM	11140		HR 667 HR 667			27. 533	1.00 10.21	В	C
ATOM	11140					27.067	1.00 15.29	В	C
ATOM	11141		HR 667 LU 668			27. 323	1.00 16.16	В	0
ATOM	11142		LU 668 LU 668			25.906	1.00 16.99	В	N
ATOM	11143		LU 668			24. 823	1.00 16.90	В	C
ATOM	11144		LU 668			23.625	1.00 17.50	В	C
ATOM	11146		LU 668	96. 275		22.867 21.850	1.00 21.31 1.00 22.06	В	C
ATOM	11147	OE1 GI		97. 284		21. 123	1.00 22.00	В	C
ATOM	11148	OE2 GI		95. 284		21.767	1.00 23.39	В	0
ATOM	11149		LU 668	98. 751	44. 127	25. 247	1.00 42.03	В	0
ATOM	11150		LU 668	99. 186		24. 766	1.00 17.77	B B	C
ATOM	11151		RG 669	99. 418		26. 158	1.00 19.28		0 N
ATOM	11152	CA AI		100. 721	44. 392	26. 640	1.00 17.02	B B	N
ATOM	11153		RG 669	101. 199		27. 785	1.00 17.00	В	C
ATOM	11154		RG 669	102. 498		28. 451	1.00 17.11	В	C C
ATOM	11155		RG 669	102. 430		29. 583	1.00 15.35	В	Č
ATOM	11156		RG 669	102. 914	47.149	29. 122		В	N
ATOM	11157	CZ AI		102.549		29. 856	1.00 16.26	В	Č
ATOM	11158	NH1 AI		102. 115	48. 023	31. 101	1.00 16.86	В	N
ATOM	11159	NH2 AF		102. 602	49.417	29. 340	1.00 14.86	В	N
ATOM	11160	C AI		100. 633	42.960	27. 140	1.00 17.70	В	Č
ATOM	11161	0 AF		101. 523	42.141	26. 899	1.00 17.72	В	ő
ATOM	11162	N TY		99. 539	42.655	27. 825	1.00 17.60	В	N
ATOM	11163	CA TY		99. 357	41.333	28. 385	1.00 16.56	В	C
ATOM	11164	CB TY		98. 823	41.465	29.810	1.00 15.82	В	Č
ATOM	11165	CG TY		99. 571	42. 491	30. 631	1.00 15.47	В	č
ATOM	11166	CD1 TY		98. 978	43. 706	30. 973	1.00 14.06	B	Č
ATOM	11167	CE1 TY		99. 680	44. 676	31.676	1.00 14.00	В	č
ATOM	11168	CD2 TY		100. 894	42. 268	31.024	1.00 14.00	В	Č
ATOM	11169	CE2 TY		101.608	43. 232	31.732	1.00 15.78	В	Č
ATOM	11170	CZ TY		100. 998	44. 433	32. 051	1.00 15.30	В	Č
ATOM	11171	OH TY		101.713		32.714	1.00 15.22	В	0
			010			25: (II	1.00 10.00	ע	U

					(Continued)
				FIG. 4-229	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	11172 11173 11174 11175 11176 11177 11178 11179 11180 11181 11182 11183 11184 11185	C TYR O TYR N MET CA MET CB MET CG MET SD MET CE MET O MET N GLY C GLY O GLY N LEU	670 670 671 671 671 671 671 671 672 672 672 672 673	98. 435 40. 441 27. 578 1. 00 17. 87 98. 637 39. 231 27. 508 1. 00 18. 02 97. 435 41. 040 26. 948 1. 00 18. 57 96. 452 40. 271 26. 199 1. 00 19. 04 95. 063 40. 844 26. 482 1. 00 21. 47 94. 604 40. 692 27. 919 1. 00 21. 74 94. 228 38. 972 28. 277 1. 00 28. 61 92. 570 38. 871 27. 582 1. 00 23. 84 96. 640 40. 164 24. 692 1. 00 19. 95 96. 121 39. 240 24. 075 1. 00 20. 85 97. 380 41. 092 24. 094 1. 00 20. 28 97. 540 41. 063 22. 654 1. 00 19. 08 96. 354 41. 807 22. 068 1. 00 21. 18	B C B O B N B C B C B C B C B C B C B C B C B C B C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	11187 11188 11189 11190 11191 11192 11193 11194 11195 11196	CA LEU CB LEU CG LEU CD1 LEU CD2 LEU C LEU O LEU N PRO CD PRO CA PRO	673 673 673 673 673 673 673 674 674	94. 884 42. 225 20. 186 1. 00 21. 44 95. 204 42. 569 18. 732 1. 00 22. 03 96. 287 43. 627 18. 507 1. 00 24. 89 1 96. 518 43. 837 17. 023 1. 00 23. 45 1 95. 846 44. 932 19. 150 1. 00 27. 67 1	3 N 3 C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	11197 11198 11199 11200 11201 11202 11203 11204 11205 11206	CB PRO CG PRO O PRO N THR CA THR CB THR OG1 THR CG2 THR C THR	674 674 674 674 675 675 675 675	90. 365 42. 347 21. 420 1. 00 19. 09 19. 09 19. 09 19. 09 19. 09 19. 09 19. 09 19. 09 19. 09 19. 09 19. 09 19. 09 19. 18. 24 19. 18. 19. 18. 19. 19. 19. 19. 19. 19. 19. 19. 19. 19	3 C 3 C 3 C 3 O 3 N 3 C 3 C 3 C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	11207 11208 11209 11210 11211 11212 11213 11214 11215 11216 11217 11218 11219 11220	O THR N PRO CD PRO CA PRO CB PRO C PRO O PRO N GLU CA GLU CB GLU CD GLU OE1 GLU	675 676 676 676 676 676 677 677 677 677	90. 825 38. 668 16. 931 1. 00 25. 46 91. 424 37. 952 17. 736 1. 00 25. 82 90. 023 38. 160 15. 991 1. 00 26. 60 89. 130 38. 885 15. 074 1. 00 25. 76 89. 823 36. 714 15. 877 1. 00 26. 64 88. 860 36. 599 14. 702 1. 00 25. 84 88. 066 37. 859 14. 801 1. 00 24. 99 91. 135 35. 967 15. 630 1. 00 28. 63 91. 347 34. 875 16. 160 1. 00 28. 85 92. 021 36. 557 14. 834 1. 00 30. 55 89. 286 35. 905 14. 534 1. 00 31. 94 89. 772 36. 290 13. 135 1. 00 35. 44 94. 177 35. 077 12. 294 1. 00 41. 76 89. 92. 984 34. 204 11. 897 1. 00 46. 15 892. 234 34. 610 10. 980 1. 00 49. 52	0

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										(Continu	(her
		•			FIG	G. 4-	230			(Continu	ieu/
ATOM	11221		GLU	677	92. 789	33. 121	12. 503	1.00 46.47	В	0	
ATOM	11222	C	GLU	677	94. 382	36.174	15. 563	1.00 31.51	В	C	
ATOM	11223	0	GLU	677	95. 565	35.938	15. 305	1.00 31.18	В	0	
ATOM	11224	N	ASP	678	94.003		16. 730	1.00 29.04	В	N	
ATOM	11225	CA	ASP	678	95.005	36.896	17. 756 17. 917	1.00 26.71 1.00 25.30	В	C	
ATOM	11226	CB	ASP	678	95. 359		18. 902	1.00 25.50	B B	C C	
ATOM ATOM	11227 11228	CG	ASP ASP	678 678	96. 500 97. 004		19. 008	1.00 20.33	В	0	
ATOM	11229		ASP	678	96. 900		19.579	1.00 24.47	В	0	
ATOM	11230	C	ASP	678	94. 586	36. 325	19. 098	1.00 25.24	В	C	
ATOM	11231	Õ	ASP	678	94. 946		19. 426	1.00 26.23	В	ŏ	
ATOM	11232	Ň	ASN	679	93. 814		19.871	1.00 24.14	B	N	
ATOM	11233	CA	ASN	679	93. 418		21. 186	1.00 22.47	B	Ċ	
ATOM	11234	CB	ASN	679	94. 456	37.089	22. 217	1.00 23.05	В	C	
ATOM	11235	CG	ASN	679	94. 390		23. 524	1.00 22.50	В	C	
ATOM	11236	0D1	ASN	679	94.644		24. 592	1.00 21.44	В	0	
ATOM	11237	ND2	ASN	679	94.059	35.037	23.448	1.00 22.30	В	N	
ATOM	11238	C	ASN	679	92.019	37.061	21.596	1.00 21.85	В	C	
ATOM	11239	0	ASN	679	91. 727	37. 174	22. 785	1.00 21.56	В	0	
ATOM	11240	N	LEU	680	91. 153	37. 316	20.619	1.00 22.96	В	N	
ATOM	11241	CA	LEU	680	89. 783	37. 750	20. 913	1.00 22.05	В	C	
ATOM	11242	CB	LEU	680	88. 999	37. 967	19.617	1.00 20.94	В	Ċ	
ATOM	11243	CG	LEU	680	87. 524	38. 379	19. 734	1.00 20.98	В	C	
ATOM	11244		LEU	680	87. 385	39. 671	20. 539	1.00 21.18	В	C	
MOTA	11245		LEU	680	86. 946	38. 567	18. 348	1.00 17.15	В	C	
ATOM ATOM	11246	C	LEU LEU	680	89. 031	36. 762	21.805	1.00 22.36	В	C	
ATOM	11247 11248	O N	ASP	680 681	88. 316 89. 193	37. 171 35. 466	22. 718	1.00 23.81 1.00 22.95	B B	O N	
ATOM	11249	CA	ASP	681	88. 502	34. 469	21. 555 22. 371	1.00 24.95	В	C	
ATOM	11250	CB	ASP	681	88. 910	33. 048	21. 980	1.00 24.73	В	C	
ATOM	11251	CG	ASP	681	88. 270	32. 587	20. 695	1.00 25.98	В	Č	
ATOM	11252		ASP	681	87. 453	33. 334	20. 116	1.00 28.21	В	ŏ	
ATOM	11253		ASP	681	88. 587	31.462	20. 259	1.00 28.60	В	Ö	
ATOM	11254	C	ASP	681	88. 754	34. 655	23. 862	1.00 23.99	B	Č	
ATOM	11255	0	ASP	681	87.816	34.640	24.660	1.00 24.77	B	Ŏ	
ATOM	11256	N	HIS	682	90.014	34.819	24. 252	1.00 22.66	B	N	
ATOM	11257	CA	HIS	682	90. 289	34.998	25.667	1.00 22.62	В	C	
ATOM	11258	CB	HIS	682	91.775	34.867	25. 981	1.00 23.03	В	C	
ATOM	11259	CG	HIS	682	92.063	34.898	27. 448	1.00 25.79	В	C	
ATOM	11260		HIS	682	92. 844	35. 718	28. 190	1.00 26.73	В	C	
ATOM	11261		HIS	682	91. 458	34. 035	28. 338	1.00 25.30	В	N	
ATOM	11262		HIS	682	91.852	34. 326	29. 565	1.00 26.50	В	C	
ATOM	11263		HIS	682	92. 693	35. 344	29. 504	1.00 26.09	В	N	
ATOM	11264	C	HIS	682	89. 775	36. 344	26. 175	1.00 21.71	В	C	
ATOM	11265	0	HIS	682	89. 412	36. 465	27. 345	1.00 20.98	В	0	
ATOM	11266	N N	TYR	683	89. 753	37. 355	25. 307	1.00 19.91	В	N	
ATOM ATOM	11267 11268	CA CB	TYR	683	89. 232	38.657	25. 707	1.00 19.50 1.00 16.55	В	C	
ATOM	11269	CG	TYR TYR	683 683	89. 226	39. 646 40. 574	24. 542	1.00 16.55	B B	C	
UIOM	11609	νu	111	UOJ	90. 419	40.014	24. 472	1.00 10.00	Ø	C	

					FIG	G. 4	231			(Continued)
ATOM ATOM			1 TYR 1 TYR	683 683	91. 616 92. 700		23. 877 23. 786	1.00 16.29 1.00 16.38	В	C ·
ATOM			2 TYR	683	90. 345	41.871	24. 980		В В	C C
ATOM	11273	CE:	2 TYR	683	91.430		24. 893	1.00 14.60	B	č
ATOM		CZ	TYR	683	92.598	42.326	24. 295	1.00 15.79	В	C
ATOM	11275	OH	TYR	683	93.663	43. 193	24. 192	1.00 16.43	В	0
ATOM ATOM	11276	C	TYR	683	87. 793	38. 437	26. 150	1.00 21.02	В	C
ATOM	11277 11278	O N	TYR ARG	683 684	87. 355 87. 071	38. 955 37. 644	27. 174 25. 367	1.00 20.95 1.00 22.94	В	0 N
ATOM	11279	CA	ARG	684	85.667	37. 349	25.634	1.00 24.94	B B	N C
ATOM	11280	CB	ARG	684	84. 992	36. 871	24. 344	1.00 24.11	В	Č
ATOM	11281	CG	ARG	684	84.996	37. 908	23. 234	1.00 25.07	B	C C
ATOM	11282	CD	ARG	684	84. 197	39. 132	23.639	1.00 25.30	В	C
ATOM	11283.	NE	ARG	684	84. 453	40. 275	22. 767	1.00 27.33	В	N
ATOM ATOM	11284 11285	CZ NILI 1	ARG ARG	684	84.126	40.344	21.480	1.00 27.26	В	C
ATOM	11286		ARG	684 684	83. 518 84. 409	39. 327 41. 443	20. 880 20. 794	1.00 27.78 1.00 26.25	B B	N N
ATOM	11287	C	ARG	684	85.401	36. 340	26. 745	1.00 20.25	В	N C
ATOM	11288	0	ARG	684	84. 275	36. 239	27. 231	1.00 26.21	В	ŏ
ATOM	11289	N	ASN	685	86.421	35.591	27.148	1.00 24.53	B	N
ATOM	11290	CA	ASN	685	86. 243	34.593	28. 201	1.00 23.44	В	C
ATOM ATOM	11291	CB	ASN	685	86.959	33. 294	27. 823	1.00 26.13	В	C
ATOM	11292 11293	CG	ASN ASN	685 685	86. 132 85. 076	32. 430	26.904	1.00 33.00	В	C
ATOM	11294		ASN	685	86. 594	31.924 32.260	27. 296 25. 667	1.00 35.72 1.00 36.03	B B	O N
ATOM	11295	C	ASN	685	86. 716	35.043	29. 575	1.00 20.60	В	C
ATOM	11296	0	ASN	685	86.472	34. 361	30. 566	1.00 20.98	В	ŏ
ATOM	11297	N	SER	686	87. 382	36.186	29.644	1.00 16.28	В	N
ATOM	11298	CA	SER	686	87. 887	36.666	30. 918	1.00 16.33	В	C
ATOM ATOM	11299 11300	CB	SER	686	89.360	37.063	30. 773	1.00 17.18	В	C
ATOM	11300	OG C	SER SER	686 686	89. 530 87. 089	38. 050 37. 837	29. 768	1.00 17.94	В	0
ATOM	11302	ŏ	SER	686	87.625	38.667	31. 486 32. 221	1.00 15.71 1.00 13.91	B B	C 0
ATOM	11303	Ň	THR	687	85. 807		31. 155	1.00 13.31	В	N N
ATOM	11304	CA	THR	687	84.989	38.992	31.655	1.00 15.19	B	Ċ
ATOM	11305	CB	THR	687	83. 899	39,401	30.639	1.00 16.80	В	C
ATOM	11306		THR	687	82. 915	38. 362	30. 537	1.00 18.14	В	0
ATOM ATOM	11307 11308	C	THR THR	687	84. 519	39.657	29. 265	1.00 16.92	В	C
ATOM	11308	Ö	THR	687 687	84. 309 84. 153	38. 605 37. 425	32. 957 33. 264	1.00 14.86	В	C
ATOM	11310	N	VAL	688	83. 910	39.616	33. 717	1.00 13.79 1.00 14.71	B B	O N
ATOM	11311	CA	VAL	688	83. 224	39.411	34. 977	1.00 14.11	В	C
ATOM	11312	CB	VAL	688	83. 239	40.691	35. 824	1.00 15.67	B	č
ATOM	11313		VAL	688	82.476	40.464	37. 130	1.00 15.43	B	č
ATOM	11314	CG2		688	84. 687	41.115	36. 100	1.00 18.49	В	C
ATOM	11315	C	VAL	688	81.777	39.048	34. 687	1.00 14.74	В	C
ATOM ATOM	11316 11317	O N	VAL Met	688 680	81.196	38. 188	35. 350	1.00 15.40	В	0
ATOM	11318	CA	MET	689 689	81. 209 79. 826	39. 710 39. 496	33. 682 33. 283	1.00 13.94	B B	N C
. 11 0111	11010	Of 1	um I	003	13.040	JJ. 4JU	JJ. 400	1.00 14.18	D	С

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						(Continued)
					FIG. 4-232	(COMBINIOU)
ATOM ATOM ATOM ATOM ATOM	11319 11320 11321 11322 11323	CB CG SD CE C	MET MET MET MET MET	689 689 689 689	79.519 40.287 32.010 1.00 14.10 79.359 41.793 32.217 1.00 18.18 80.817 42.684 32.849 1.00 21.67 81.693 43.067 31.308 1.00 19.11 79.429 38.040 33.080 1.00 13.66	B C B C B S B C
ATOM ATOM	11324 11325	O N	MET SER	689 690	78. 398 37. 597 33. 586 1. 00 14. 01 80. 246 37. 290 32. 356 1. 00 14. 32	B C B O B N
ATOM ATOM ATOM	11326 11327 11328	CA CB OG	SER SER SER	690 690 690	79. 939 35. 887 32. 087 1. 00 16. 68 81. 018 35. 259 31. 199 1. 00 18. 28	B C B C
ATOM ATOM	11329 11330	C 0	SER SER	690 690	82. 225	B O B C B O
ATOM	11331	N	ARG	691	80. 238 35. 502 34. 478 1. 00 14. 35	B N
ATOM	11332	CA	ARG	691	80. 155 34. 741 35. 727 1. 00 15. 38	B C
ATOM	11333	CB	ARG	691	81. 491 34. 821 36. 478 1. 00 16. 76	B C
ATOM	11334	CG	ARG	691	82. 697 34. 414 35. 652 1. 00 19. 96	B C
ATOM	11335	CD	ARG	691	83. 972 34. 339 36. 483 1. 00 21. 36	B C
ATOM	11336	NE	ARG	691	85. 061 33. 725 35. 726 1. 00 23. 56	B N
ATOM	11337	CZ	ARG	691	86. 196 33. 274 36. 256 1. 00 26. 24	B C
ATOM	11338	NH1	ARG	691	86. 418 33. 358 37. 567 1. 00 23. 55	B N
ATOM ATOM ATOM	11339 11340 11341	NH2 C		691 691	87. 114 32. 728 35. 468 1. 00 26. 33 79. 049 35. 187 36. 679 1. 00 15. 48	B N B C
ATOM ATOM	11342 11343	O N CA	ALA ALA	691 692 692	78. 986 34. 713 37. 817 1. 00 14. 38 78. 178 36. 081 36. 220 1. 00 14. 78 77. 111 36. 618 37. 064 1. 00 16. 42	B O B N B C
ATOM	11344	CB	ALA	692	76. 105 37. 383 36. 198 1. 00 16. 75 76. 375 35. 624 37. 977 1. 00 17. 17 76. 331 35. 814 39. 191 1. 00 16. 75	B C
ATOM	11345	C	ALA	692		B C
ATOM	11346	0	ALA	692		B O
ATOM	11347	N	GLU	693	75. 803 34. 571 37. 404 1. 00 19. 44	B N
ATOM	11348	CA	GLU	693	75. 062 33. 589 38. 191 1. 00 22. 16	B C
ATOM	11349	CB	GLU	693	74. 570 32. 443 37. 299 1. 00 26. 71 73. 251 32. 745 36. 598 1. 00 33. 79 73. 017 31. 873 35. 379 1. 00 38. 47	B C
ATOM	11350	CG	GLU	693		B C
ATOM	11351	CD	GLU	693		B C
ATOM ATOM ATOM	11352 11353 11354		GLU GLU GLU	693 693 693	72. 984 30. 632 35. 531 1. 00 40. 41 72. 870 32. 433 34. 266 1. 00 41. 15	B 0 B 0
ATOM ATOM	11355 11356	O N	GLU ASN	693 694	75. 244 32. 761 40. 418 1. 00 24. 44 77. 127 32. 824 39. 215 1. 00 21. 66	B C B O B N
ATOM	11357	CA	ASN	694	77. 907 32. 282 40. 320 1. 00 22. 61 79. 324 31. 924 39. 861 1. 00 20. 93 79. 359 30. 654 39. 048 1. 00 19. 32	B C
ATOM	11358	CB	ASN	694		B C
ATOM	11359	CG	ASN	694		B C
ATOM	11360	OD1	ASN	694	80. 284 30. 420 38. 278 1. 00 19. 68	B O
ATOM	11361	ND2	ASN	694	78. 348 29. 818 39. 224 1. 00 18. 34	B N
ATOM	11362	C	ASN	694	77. 975 33. 234 41. 500 1. 00 22. 99 78. 650 32. 946 42. 479 1. 00 25. 59 77. 283 34. 366 41. 419 1. 00 22. 83	B C
ATOM	11363	O	ASN	694		B O
ATOM	11364	N	PHE	695		B N
ATOM	11365	CA	PHE	695	77. 299 35. 316 42. 531 1. 00 23. 74	B C
ATOM	11366	CB	PHE	695	77. 205 36. 772 42. 041 1. 00 20. 88	B C
ATOM	11367	CG	PHE	695	78. 533 37. 397 41. 695 1. 00 19. 06	B C

					FΙ	G. 4	- 233			(Continued)
ATOM	11368		PHE	695	79. 211			1.00 19.50	В	С
ATOM	11369		PHE	695	79.096			1.00 19.69	В	Č
ATOM	11370		PHE	695	80. 431			1.00 18.29	В	C
ATOM Atom	11371		PHE PUR	695	80.316			1.00 18.53	В	C
ATOM	11372 11373	CZ C	PHE PHE	695	80.982		41.033	1.00 17.35	В	C
ATOM	11374	0	PHE	695 695	76.146			1.00 24.37	В	C
ATOM	11374	N	LYS	696	76.090		44. 566	1.00 25.67	В	0
ATOM	11376	CA	LYS	696	75. 230 74. 074		43. 089 43. 926	1.00 24.40	В	N ·
ATOM	11377	CB	LYS	696	73. 173		43. 280	1.00 25.82 1.00 27.75	В	C
ATOM	11378	CG	LYS	696	72. 076		44. 228	1.00 21.73	B B	C C C
ATOM	11379	CD	LYS	696	70. 680		43. 615	1.00 30.02	В	C
ATOM	11380	CE	LYS	696	70.137		43. 421	1.00 31.03	В	Č
ATOM	11381	NZ	LYS	696	69.903		44. 705	1.00 35.47	. В	N
ATOM	11382	C	LYS	696	74. 402		45. 348	1.00 24.85	В	Č
ATOM	11383	0	LYS	696	73.583		46. 242	1.00 24.94	В	ő
ATOM	11384	N	GLN	697	75.587	32.907	45. 577	1.00 25.99	B	N
ATOM	11385	CA	GLN	697	75.920	32.481	46.931	1.00 27.33	$\tilde{\mathbf{B}}$	Ċ
ATOM	11386	CB	GLN	697	76.355	31.010	46.941	1.00 29.90	B	Č
ATOM	11387	CG	GLN	697	75. 290	30.025	46. 444	1.00 30.66	В	Č
ATOM	11388	CD	GLN	697	75.565	28. 593	46.889	1.00 30.92	В	C
ATOM	11389		GLN	697	75.381	28. 245	48.065	1.00 31.54	В	0
ATOM	11390		GLN	697	76.019	27. 761	45.958	1.00 26.21	В	N
ATOM	11391	C	GLN	697	76.964	33. 322	47.662	1.00 26.04	В	C
ATOM	11392	0	GLN	697	77. 620	32.833	48. 580	1.00 28.31	В	0
ATOM	11393	N	VAL	698	77. 125	34. 580	47. 270	1.00 23.16	В	N
ATOM	11394	CA	VAL	698	78. 085	35. 445	47. 947	1.00 21.23	В	C
ATOM ATOM	11395 11396	CB	VAL	698	79. 411	35. 596	47. 156	1.00 20.63	В	Č
ATOM	11390	CG1		698	80. 033	34. 238	46. 901	1.00 17.19	В	C
ATOM	11398	C	VAL VAL	698	79.161	36. 335	45. 853	1.00 18.36	В	C
ATOM	11399	Ö	VAL	698 698	77. 496	36. 829	48.118	1.00 21.50	В	C
ATOM	11400	N	GLU	699	76. 571 78. 018	37. 207 37. 579	47. 404	1.00 23.06	В	0
ATOM	11401	CA	GLU	699	77. 563	38. 945	49. 078 49. 290	1.00 21.31 1.00 21.42	В	N
ATOM	11402	CB	GLU	699	77. 465	39. 246	50. 785	1.00 21.42	В	C
ATOM	11403	CG	GLU	699	76. 396	38. 403	51.461	1.00 22.13	B B	C
ATOM	11404	CD	GLU	699	76.547	38. 346	52. 961	1.00 29.09	В	C C
ATOM	11405		GLU	699	76. 343	39. 387	53. 624	1.00 23.03	В	.0
ATOM	11406		GLU	699	76.876	37. 254	53. 476	1.00 31.23	В	.0
ATOM	11407	C	GLU	699	78.610	39.810	48. 593	1.00 21.23	B	Č
ATOM	11408	0	GLÜ	699	79. 802	39. 751	48. 905	1.00 21.45	В	ŏ
ATOM	11409	N	TYR	700	78. 148	40. 594	47.630	1.00 19.47	B	Ň
ATOM	11410	CA	TYR	700	79.012	41.428	46.818	1.00 18.26	В	Č
ATOM	11411	CB	TYR	700	78.830	41.001	45. 368	1.00 18.24	B	č
ATOM	11412	CG	TYR	700	79.678	41.685		1.00 18.56	B	·Č
ATOM	11413	CD1		700	81.071	41.698	44.422	1.00 17.75	B	Č
ATOM	11414	CE 1		700	81.856	42. 206	43. 378	1.00 17.99	B	Č
ATOM	11415	CD2		700	79.088	42. 209	43. 181	1.00 19.07	В	Č
ATOM	11416	CE2	TYR	700	79.852	42.715	42. 143	1.00 19.54	В	Č

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					D		00-			(Continued)
					FIG	·. 4 ·	2 3 5			
ATOM			ALA		83. 114	59. 741	37. 739	1.00 13.21	В	N
ATOM				707	84.075	60.522	36.969	1.00 14.57	В	C
ATOM ATOM				707	84. 277	61.881	37. 626	1.00 17.64	В	C
ATOM			ALA ALA	707 707	85. 427 86. 445	59.823	36. 802	1.00 13.77	В	C
ATOM			ASP	708	85. 435	60. 484 58. 494	36. 639 36. 839	1.00 14.15 1.00 13.35	B B	0 N
ATOM				708	86. 667	57. 721	36. 685	1.00 13.35	В	N C
ATOM			ASP	708	86. 439	56. 285	37. 188	1.00 12.24	В	Č
ATOM				708	87. 737	55.536	37.453	1.00 10.05	В	Č
ATOM			1 ASP	708	88. 738	55.775	36. 749	1.00 11.19	В	0
ATOM ATOM			2 ASP ASP	708		54.686	38. 362	1.00 9.31	В	0
ATOM			ASP	708 708		57. 696 57. 023	35. 202	1.00 13.18	В	C
ATOM	11479		ASP	709		58. 423	34. 368 34. 891	1.00 13.78 1.00 12.80	B B	0
ATOM	11480		ASP	709		58. 520	33. 534	1.00 12.65	В	N C
ATOM	11481	CB	ASP	709		59.825	33. 397	1.00 11.74	В	Č
ATOM	11482	CG	ASP	709	90.612	59.912	34.366	1.00 9.63	B	č
ATOM	11483		ASP	709		59.385	34.058	1.00 2.39	В	0
ATOM ATOM	11484 11485	C	ASP ASP	709		60.499	35. 451	1.00 11.84	В	0
ATOM	11486	0	ASP	709 709		57. 366 57. 136	33. 167	1.00 14.57	В	C
ATOM	11487	N	ASN	710		56.652	31. 987 34. 182	1.00 16.47 1.00 13.58	В В	O N
ATOM	11488	CA	ASN	710		55. 524	33. 990	1.00 13.56	В	C
ATOM	11489	CB	ASN	710		55. 385	35. 243	1.00 13.26	В	Č
ATOM	11490	CG	ASN	710	92. 987	54. 440	35.059	1.00 12.07	B	č
ATOM ATOM	11491		ASN	710		54. 478	35.821	1.00 16.69	В	0
ATOM	11492 11493	RDZ C	ASN ASN	710		53. 578	34. 058	1.00 8.28	В	N
ATOM	11494	0	ASN	710 710		54. 236 53. 737		1.00 14.26	В	C
ATOM	11495	Ň	VAL	711		53. 692	32. 598 34. 773	1. 00 14. 29 1. 00 13. 24	В	0
ATOM	11496	CA	VAL	711		52. 511	34. 652	1.00 13.24	B B	N C
ATOM	11497	CB	VAL	711		51.585	35. 868	1.00 11.72	В	C
ATOM	11498	CG1	VAL	711	88. 048	50. 311	35.624	1.00 7.36	·B	č
ATOM	11499		VAL	711		51. 274	36. 141	1.00 13.94	В	Č
ATOM Atom	11500 11501	C 0	VAL VAL	711	87. 315	3. 119	34. 645	1.00 14.01	В	С
ATOM	11501	N	HIS	711 712		3. 471	35. 694	1.00 13.52	В	0
ATOM	11503	CA	HIS	712		53. 249 53. 869	33. 456 33. 290	1.00 13.66 1.00 13.44	В	N
ATOM	11504	CB	HIS	712		3. 956		1.00 13.44	B B	C C
ATOM	11505	CG.	HIS	712		4.613	31.001	1.00 14.38	В	C .
ATOM	11506		HIS	712	87. 137 5	5. 549		1.00 15.50	B	Č
ATOM	11507		HIS	712		4. 299	29. 684	1.00 15.76	В	Ň
ATOM ATOM	11508 11509		HIS HIS	712				1.00 17.42	В	C
ATOM	11510	C	HIS	712 712				1.00 16.57	В	N
ATOM	11511	0	HIS	712				1.00 13.09	В	C
ATOM	11512	Ň	PHE	713				1.00 13.25 1.00 13.27	В	0
ATOM	11513	CA	PHE	713				1.00 15.27	B B	N C
ATOM	11514	CB	PHE	713	.			1.00 15.17	В	C

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					F 1. (G. 4-	236			(Continued	l)
ATOM	11515	CG	PHE	713	80. 156	54. 464	36.461	1.00 16.61	В	С	
ATOM	11516		PHE	713	80. 346	54. 508	37. 841	1.00 14.51	В	C	
ATOM	11517		PHE	713	78. 901	54.111	35. 962	1.00 15.42	В	Č	
ATOM	11518		PHE	713	79. 304	54. 204	38. 710	1.00 14.71	В	Č	
ATOM	11519		PHE	713	77. 848	53. 803	36. 829	1.00 15.24	B	Č	
ATOM	11520	CZ	PHE	713	78.051	53.849	38. 204	1.00 13.41	B	Č	
ATOM	11521	Č	PHE	713	81.586	52.486	34. 499	1.00 16.62	В	Ċ	
ATOM	11522	0	PHE	713	81.015	51.527	35.031	1.00 16.48	В	0	
ATOM	11523	N	GLN	714	81.673	52.649	33. 181	1.00 15.73	В	N	
ATOM	11524	CA	GLN	714	81.121	51.699	32.228	1.00 16.08	В	С	
ATOM	11525	CB	GLN	714	81.753	51.923	30.857	1.00 14.90	В	C	
ATOM	11526	CG	GLN	714	81.699	50.703	29.946	1.00 16.13	В	С	
ATOM	11527	CD	GLN	714	82.661	50.811	28.770	1.00 15.37	В	С	
ATOM	11528	0E1	GLN	714	83. 821	51.167	28. 943	1.00 15.11	В	0	
ATOM	11529		GLN	714	82.183	50.493	27.577	1.00 15.35	В	N	
ATOM	11530	C	GLN	714	81.372	50.256	32.650	1.00 16.29	В	C	
ATOM	11531	0	GLN	714	80. 512	49.389	32. 487	1.00 17.82	В	0	
ATOM	11532	N	GLN	715	82. 554	49.997	33. 192	1.00 14.60	В	N	
ATOM	11533	CA	GLN	715	82.900	48.646	33. 593	1.00 14.55	В	C	
ATOM	11534	CB	GLN	715	84. 395	48. 581	33. 926	1.00 16.22	В	C	
ATOM	11535	CG	GLN	715	85. 270	49.086	32.767	1.00 16.01	В	C	
ATOM	11536	CD	GLN	715	86. 507	48. 247	32. 537	1.00 14.28	В	C	
ATOM ATOM	11537	OE1	GLN	715	86.470	47.029	32.674	1.00 17.54	В	0	
ATOM	11538 11539	C	GLN GLN	715 715	87. 601 82. 031	48. 889 48. 134	32. 155 34. 746	1.00 12.78	В	N	
ATOM	11540	0	GLN	715	81.616	46. 134	34. 749	1.00 14.99 1.00 13.70	В	C	
ATOM	11540	N	SER	716	81.742	49.002	34. 749 35. 714	1.00 13.70	B B	. N	
ATOM	11542	CA	SER	716	80. 893	48.602	36. 829	1.00 12.14	В	C	
ATOM	11543	CB	SER	716	81.057	49.544	38. 028	1.00 11.10	В	C	
ATOM	11544	0G	SER	716	82. 278	49. 295	38. 700	1.00 13.48	В	Ö	
ATOM	11545	Č	SER	716	79. 432	48. 570	36. 394	1.00 9.18	В	Č	
ATOM	11546	Ŏ	SER	716	78. 682	47.692	36. 814	1.00 5.81	В	ŏ	
ATOM	11547	Ň	ALA	717	79. 026	49.517	35. 552	1.00 8.69	B	N	
ATOM	11548	CA	ALA	717	77. 639	49.537	35.083	1.00 10.91	B	Ċ	
ATOM	11549	CB	ALA	717	77.400	50.708	34. 143	1.00 10.07	B	Č	
ATOM	11550	C	ALA	717	77.304	48. 219	34. 382	1.00 10.72	В	Ċ	
ATOM	11551	0	ALA	717	76. 212	47.696	34.539	1.00 14.08	В	0	
ATOM	11552	N	GLN	718	78. 252	47.682	33.623	1.00 10.89	В	N	
ATOM	11553	CA	GLN	718	78.052	46.417	32.928	1.00 10.32	В	С	
ATOM	11554	CB	GLN	718	79. 137	46. 224	31.858	1.00 8.83	В	C	
ATOM	11555	CG	GLN	718	79.074	47. 232	30. 722	1.00 6.53	В	С	
ATOM	11556	CD	GLN	718	78.002	46.900	29.691	1.00 8.70	В	C	
ATOM	11557	0E1		718	76.970	46.319	30.012	1.00 13.43	В	0	
ATOM	11558	NE2		718	78. 243	47. 278	28. 449	1.00 11.12	В	N	
ATOM	11559	C	GLN	718	78.056	45. 235	33. 908	1.00 10.68	В	Č	
ATOM	11560	0	GLN	718	77. 357	44. 248	33. 695	1.00 13.48	В	0	
ATOM	11561	N	ILE	719	78. 834	45. 320	34. 981	1.00 12.24	В	N	
ATOM	11562	CA	ILE	719	78. 851	44. 226	35. 953	1.00 12.41	В	Č	
ATOM	11563	CB	ILE	719	79.892	44. 434	37.079	1.00 12.88	В	C	

						(Continued)
					FIG. 4-237	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	11564 11565 11566 11567 11568 11570 11571 11573 11574 11575 11576 11576 11577 11580 11581 11582 11583 11584 11585 11586 11587 11588 11589 11590 11591 11592 11593 11594 11595 11597 11598 11599 11600 11601 11602	CGCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	ILE ILE SER SER LYS SER LYS LYS ALA ALA ALA LEU LEU VAL LEU VAL	719 719 719 719 719 720 720 720 720 720 721 721 721 721 721 721 722 722 722 722	79. 550 43. 532 38. 266 1. 00 9. 78 B 81. 302 44. 131 36. 560 1. 00 13. 61 B 82. 383 44. 146 37. 643 1. 00 12. 97 B 77. 494 44. 134 36. 621 1. 00 12. 95 B 76. 932 43. 049 36. 757 1. 00 13. 41 B 76. 979 45. 286 37. 043 1. 00 12. 96 B 75. 694 45. 345 37. 716 1. 00 13. 07 B 75. 418 46. 771 38. 211 1. 00 12. 56 B 75. 435 47. 716 37. 147 1. 00 15. 69 B 74. 558 44. 865 36. 814 1. 00 14. 11 B 73. 712 44. 073 37. 238 1. 00 13. 45 B 74. 536 45. 329 35. 569 1. 00 12. 91 B 73. 474 44. 919 34. 664 1. 00 14. 17 B 72. 241 46. 368 31. 378 1. 00 10	(Continued) C C C C C C C C C C C C C C C C C C
ATOM	11601	CG2	VAL	724	70. 479 44. 487 38. 213 1. 00 19. 61 B	C .
ATOM ATOM	11603 11604	0 N	VAL ASP	724 725	68. 824 40. 441 36. 800 1. 00 16. 03 B 70. 509 40. 920 35. 391 1. 00 19. 41 B	O N
ATOM ATOM	11605 11606	CA CB	ASP ASP	725 725	70. 015 39. 999 34. 379 1. 00 21. 58 B 70. 965 39. 930 33. 191 1. 00 23. 71 B	C C
ATOM ATOM	11607 11608	CG OD1		725 725	70. 957 41. 197 32. 372 1. 00 27. 35 B 69. 919 41. 895 32. 368 1. 00 27. 29 B	C 0
ATOM ATOM	11609 11610	OD2 C	ASP	725 725	71. 983 41. 486 31. 717 1. 00 31. 72 B 69. 748 38. 591 34. 893 1. 00 22. 63 B	0 C
ATOM ATOM	11611 11612	O N	ASP VAL	725 726	68. 763 37. 974 34. 474 1. 00 24. 48 B 70. 607 38. 075 35. 781 1. 00 20. 53 B	O N
					NIDOTITUTE OURSE (S. V. S. C.)	

										(Continued	()
					FIG	r. 4 -	238			(002000	
		٠.						1 00 17 09	n	C	
ATOM	11613	CA	VAL	726	70.409	36. 726	36. 329 36. 392	1.00 17.93 1.00 19.28	B B	C C C	
ATOM	11614	CB	VAL	726	71.727	35. 920 35. 672	34. 994	1.00 19.28	В	Č	
ATOM	11615		VAL	726 726	72. 246 72. 763	36.660	37. 238	1.00 19.33	В	C	
ATOM ATOM	11616 11617	CG2 C	VAL	726	69. 789	36. 741	37. 723	1.00 13.00	В	Č	
ATOM	11618	0	VAL	726	69. 858	35. 756	38. 463	1.00 16.63	В	ŏ	
ATOM	11619	N	GLY	727	69.198	37. 875	38. 081	1.00 17.14	В	Ň	
ATOM	11620	CA	GLY	727	68. 548	38. 012	39. 370	1.00 15.42	B	Ĉ	
ATOM	11621	C	GLY	727	69. 387	37. 856	40.626	1.00 15.90	В	С	
ATOM	11622	ŏ	GLY	727	68.961	37. 182	41.559	1.00 17.97	В	0	
ATOM	11623	N	VAL	728	70.568	38.462	40.675	1.00 15.07	В	N	
ATOM	11624	CA	VAL	728	71.389	38.357	41.876	1.00 14.10	В	C	
ATOM	11625	CB	VAL	728	72.859	37.972	41.574	1.00 14.97	В	C	
ATOM	11626	CG1		728	73. 693	38. 145	42.829	1.00 13.51	В	C	
ATOM	11627	CG2		728	72.954	36.514	41.109	1.00 15.40	В	C	
ATOM	11628	C	VAL	728	71.396	39. 687	42.603	1.00 14.73	В	C	
ATOM	11629	0	VAL	728	71.738	40.714	42.025	1.00 14.56	В	0	
ATOM	11630	N	ASP	729	71.007	39.672	43.872	1.00 15.13	В	N C	
ATOM	11631	CA	ASP	729	70.998	40.896	44.646 45.903	1.00 15.32 1.00 15.31	B B	C C	
ATOM	11632 11633	CB CG	ASP ASP	729 729	70. 146 70. 034	40. 731 42. 019	46.696	1.00 13.31	В	C	
ATOM ATOM	11634		ASP	729	69.663	43.055	46.104	1.00 20.57	В	0	
ATOM	11635	0D1		729	70. 317	42.011	47.907	1.00 20.06	В	Ŏ	
ATOM	11636	C	ASP	729	72. 441	41.185	45.021	1.00 16.27	B	č	
ATOM	11637	ŏ	ASP	729	73. 253	40. 270	45.117	1.00 17.70	B	0	
ATOM	11638	Ň	PHE	730	72.772	42.454	45.211	1.00 16.74	В	N	
ATOM	11639	CA	PHE	730	74. 136	42.824	45.579	1.00 16.43	В	C	
ATOM	11640	CB	PHE	730	75.061	42.734	44.361	1.00 13.47	В	C	
ATOM	11641	CG	PHE	730	74. 744	43.728	43.304	1.00 12.81	В	C	
ATOM	11642		PHE	730	75. 282	45.006	43.355	1.00 12.64	В	C	
ATOM	11643		PHE	730	73. 828	43. 423	42.303	1.00 12.46	В	C	
ATOM	11644		PHE	730	74.907	45.966	42. 432	1.00 11.61	В	C	
ATOM	11645		PHE	730	73.446	44. 377	41.376	1.00 9.11	B B	C C	
ATOM	11646	CZ	PHE	730	73.986	45.653 44.242	41. 443 46. 114	1.00 10.39 1.00 17.87	В	C	
ATOM ATOM	11647 11648	C 0	PHE PHE	730 730	74. 112 73. 094	44. 242	46.014	1.00 17.87	В	Ö	
ATOM	11649	N	GLN	731	75. 230	44. 673	46.689	1.00 13.12	В	N	
ATOM	11650	CA	GLN	731	75. 344	46.015	47. 246	1.00 17.25	B	Ċ	
ATOM	11651	CB	GLN	731	76.089	45.961	48.569	1.00 18.02	B	č	
ATOM	11652	CG	GLN	731	75. 547	44. 948	49.536	1.00 25.59	B	Č	
ATOM	11653	CD	GLN	731	74.087	45. 183	49.854	1.00 29.48	В	C	
ATOM	11654	0E1	GLN	731	73. 699	46. 275	50. 281	1.00 31.32	В	0	
ATOM	11655	NE2	GLN	731	73. 263	44. 157	49.647	1.00 32.13	В	N	
ATOM	11656	C	GLN	731	76. 124	46.889	46.272	1.00 16.69	В	Ç	
ATOM	11657	0	GLN	731	77.060	46.417	45.623	1.00 13.71	В	0	
ATOM	11658	N	ALA	732	75. 737	48. 158	46. 172	1.00 15.59	В	N	
ATOM	11659	CA	ALA	732	76. 425	49.084	45. 284	1.00 15.79	В	C	
ATOM	11660	CB	ALA	732	75. 718	49.147	43.946	1.00 15.47	В	C	
MOTA	11661	C	ALA	732	76. 540	50. 486	45.867	1.00 17.21	В	C	

				FIG. 4-239	(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	11662 11663 11664 11665 11666 11667 11668 11670 11671 11672 11673 11674 11675 11677 11678 11677 11678 11680 11681 11682 11683 11684	O ALA N MET CA MET CB MET CG MET SD MET CE MET O MET N TRP CA TRP CB TRP CB TRP CC2 TRP CC2 TRP CC3 TRP CC1 TRP NE1 TRP CZ2 TRP CZ3 TRP	732 733 733 733 733 733 733 734 734 734 734	75. 769 50. 897 46. 734 1. 00 17. 93 B 77. 528 51. 220 45. 382 1. 00 17. 27 B 77. 737 52. 587 45. 812 1. 00 17. 39 B 78. 500 52. 628 47. 136 1. 00 18. 98 B 78. 775 54. 028 47. 661 1. 00 18. 20 B 77. 278 54. 979 47. 988 1. 00 21. 42 B 76. 781 54. 324 49. 578 1. 00 19. 12 B 78. 539 53. 268 44. 719 1. 00 17. 47 B 79. 604 52. 783 44. 318 1. 00 17. 30 B 78. 007 54. 378 44. 220 1. 00 16. 37 B 78. 673 55. 147 43. 175 1. 00 15. 48 B 77. 685 55. 428 42. 033 1. 00 14. 82 B 76. 691 56. 523 42. 353 1. 00 14. 06 B 75. 299 56. 363 42. 650 1. 00 12. 49 B 74. 785 57. 645 42. 939 1. 00 12. 15 B 74. 437 55. 259 42. 701 1. 00 12. 01 B 76. 953 57. 857 42. 468 1. 00 12. 61 B 75. 817 58. 535 42. 821 1. 00 13. 60 B 73. 115 55. 466 43. 034 1. 00 13. 39 B 72. 629 56. 762 43. 319 1. 00 13. 13 B 79. 111 56. 457 43. 831 1. 00 13. 60 B 78. 491 56. 881 44. 788 1. 00 14. 71	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	11685 11686 11687 11688 11690 11691 11692 11693 11694 11695 11696 11697 11698 11700 11701 11702 11703 11704 11705 11706 11707 11708	N TYR CA TYR CB TYR CG TYR CD1 TYR CE1 TYR CD2 TYR CE2 TYR CC TYR OH TYR C TYR O TYR N THR CA THR CA THR CG	735 735 735 735 735 735 735 735 735 736 736 736 736 736 737 737	80. 174 57. 090 43. 346 1. 00 13. 31 B 80. 598 58. 366 43. 926 1. 00 12. 17 B 81. 990 58. 260 44. 575 1. 00 10. 49 B 81. 964 57. 577 45. 920 1. 00 10. 18 B 81. 464 58. 232 47. 045 1. 00 11. 23 B 81. 321 57. 567 48. 272 1. 00 11. 72 B 82. 336 56. 241 46. 052 1. 00 11. 30 B 82. 198 55. 567 47. 270 1. 00 11. 75 B 81. 687 56. 235 48. 372 1. 00 12. 02 B 81. 511 55. 564 49. 563 1. 00 12. 02 B 81. 391 59. 393 41. 910 1. 00 13. 79 B 80. 595 59. 430 42. 845 1. 00 14. 20 B 81. 391 59. 393 41. 910 1. 00 15. 56 B 79. 669 60. 372 42. 977 1. 00 15. 66 B 79. 517 61. 459 42. 026 1. 00 14. 01 B 78. 395 <	0 N C C C C C C C C C C C C C C C C C C
ATOM ATOM	11709 11710	OD2 ASP C ASP	737 737	80. 680 66. 525 40. 078 1. 00 19. 23 B 83. 737 62. 811 40. 912 1. 00 15. 17 B	0 C

				E I C	4 - 2 4 0			(Continu	ued)
			•	FIG.	4 - 2 4 0				
ATOM	11711	0 ASP	737		. 560 40. 882	1.00 14.33	В	0	
ATOM	11712	N GLU	738		. 603 41. 453	1.00 14.73	В	N	
ATOM	11713	CA GLU	738		. 112 41. 986 . 208 43. 206	1.00 14.51	B B	C	
ATOM ATOM	11714 11715	CB GLU CG GLU	738 738		. 208 43. 206 . 935 44. 448	1.00 15.23 1.00 16.91	В	C C	•
ATOM	11716	CD GLU	738		. 958 44. 956	1.00 10.31	В	C	
ATOM	11717	OE1 GLU	738		.580 45.222	1.00 19.02	В	ŏ	
ATOM	11718	OE2 GLU	738		. 142 45: 100	1.00 19.97	B	ŏ	
ATOM	11719	C GLU	738		.319 40.867	1.00 13.36	В	Č	
ATOM	11720	0 GLU	738		. 763 40. 005	1.00 13.24	В	0	
ATOM	11721	N ASP	739		. 275 40. 858	1.00 12.47	В	N	
ATOM	11722	CA ASP	739		. 522 39. 824	1.00 12.05	В	C C C	
ATOM	11723	CB ASP	739		. 369 39. 166	1.00 12.46	В	C	
ATOM	11724	CG ASP	739		.717 40.101	1.00 16.27	В	C	
ATOM	11725	OD1 ASP	739		. 653 39. 751	1.00 16.93	B B	0	
ATOM ATOM	11726 11727	OD2 ASP C ASP	739 739		. 066 41. 158 . 187 40. 351	1.00 16.75 1.00 13.65	В	0 C	
ATOM	11728	0 ASP	739		. 686 41. 372	1.00 13.03	В	0	
ATOM	11729	N HIS	740		. 609 39. 661	1.00 14.00	В	N .	
ATOM	11730	CA HIS	740		. 311 40. 041	1.00 12.91	B	Č	
ATOM	11731	CB HIS	740		. 872 39. 035	1.00 12.28	B	Č	
ATOM	11732	CG HIS	740		. 418 39. 105	1.00 12.12	В	C C C	
ATOM	11733	CD2 HIS	740		. 763 39. 179	1.00 12.56	В	C	
ATOM	11734	ND1 HIS	740		. 449 39. 081	1.00 12.00	В	N	
ATOM	11735	CE1 HIS	740		. 256 39. 136	1.00 11.97	В	C	
ATOM	11736	NE2 HIS	740		. 419 39. 194	1.00 12.98	В	N	
ATOM ATOM	11737 11738	C HIS O HIS	740 740		. 209 41. 447 . 133 42. 041	1.00 14.77	В	C	
ATOM	11739	N GLY	741		. 320 41. 986	1.00 16.10 1.00 14.45	B B	O N	
ATOM	11740	CA GLY	741		. 271 43. 311	1.00 14.43	В	C	
ATOM	11741	C GLY	741		572 44.431	1.00 13.32	В	Č	
ATOM	11742	0 GLY	741		445 45.590	1.00 16.71	B	ŏ	
ATOM	11743	N ILE	742		. 946 44. 103	1.00 14.08	B	N	
ATOM	11744	CA ILE	742		. 298 45. 111	1.00 14.39	В	С	
ATOM	11745	CB ILE	742		. 082 45. 520	1.00 14.12	В	C	
ATOM	11746	CG2 ILE	742		. 539 46. 345	1.00 13.12	В	C	
ATOM	11747	CG1 ILE	742		336 44. 273	1.00 13.94	В	C	
ATOM	11748	CD1 ILE	742		214 44.553	1.00 10.86	В	C	
ATOM ATOM	11749 11750	C ILE O ILE	742		827 46.335	1.00 15.89	В	C	
ATOM	11751	N ALA	742 743		. 350 47. 453 . 828 46. 108	1.00 17.67 1.00 16.48	B B	O N	
ATOM	11752	CA ALA	743		381 47.157	1.00 10.46	В	C	
ATOM	11753	CB ALA	743		508 46.651	1.00 16.86	В	č	
ATOM	11754	C ALA	743		689 47.779	1.00 16.53	В	Č	
ATOM	11755	0 ALA	743		153 48.711	1.00 18.69	B	ŏ	
ATOM	11756	N SER	744		312 47. 287	1.00 14.28	B	Ň	
ATOM	11757	CA SER	744	88. 681 63.	556 47.908	1.00 14.62	В	C	
ATOM	11758	CB SER	744		059 47.321	1.00 16.50	В	С	
ATOM	11759	OG SER	744	86. 314 63.	152 47.573	1.00 22.09	В	0 .	

										(Continued)
					FIC	G. 4-	241			(5 5
ATOM	11760	С	SER	744	88. 515	63. 251	49. 390	1.00 15.05	В	С
ATOM	11761	0	SER		88. 136	62.147	49.770	1.00 17.03	B	0
ATOM	11762	N	SER		88. 822	64. 223	50. 229	1.00 16.05	В	N
ATOM	11763	CA	SER		88. 712	64.051	51.666	1.00 15.38	В	Ċ
ATOM	11764	CB	SER		88. 811	65.410	52.361	1.00 15.23	В	C
ATOM	11765	0G	SER	745	88. 357	65.318	53.698	1.00 20.36	В	0
ATOM	11766	C	SER		87.427	63.360	52.103	1.00 14.58	В	C
ATOM	11767	0	SER		87.467	62.334	52.773	1.00 15.64	В	0
ATOM	11768	N	THR	746	86. 287	63.925	51.728	1.00 13.39	В	N
ATOM	11769	CA	THR	746	85.009	63.355	52.121	1.00 12.46	В	C
ATOM	11770	CB	THR	746	83. 836	64.299	51.755	1.00 13.02	В	C
ATOM	11771	0G1	THR	746	83. 858	64.579	50.347	1.00 12.13	В	0
ATOM	11772	CG2			83. 929	65.599	52.547	1.00 6.36	В	C
ATOM	11773	C	THR		84. 748	61.982	51.513	1.00 13.71	В	C
ATOM	11774	0	THR		84.382	61.045	52. 215	1.00 13.77	В	0
ATOM	11775	N	ALA		84.948	61.852	50. 211	1.00 15.70	В	N
ATOM	11776	CA	ALA		84.698	60.575	49.556	1.00 17.75	В	C C
ATOM	11777	CB	ALA		84.918	60.698	48.047	1.00 18.85	В	C
ATOM	11778	C	ALA		85. 579	59. 482	50. 133	1.00 16.94	В	C
ATOM	11779	0	ALA		85. 136	58.344	50.314	1.00 17.92	В	0
ATOM	11780	N	HIS	748	86.828	59.829	50.418	1.00 15.98	В	N
ATOM	11781	CA	HIS	748	87.772	58. 873	50.987	1.00 15.53	В	C
ATOM	11782	CB	HIS	748	89.130	59. 547	51.194	1.00 14.50	В	C
ATOM	11783	CG	HIS	748	90.106	58. 721	51.974	1.00 12.65	В	C C
ATOM	11784		HIS	748	90.772	58. 979	53. 124	1.00 12.46	В	
ATOM	11785		HIS	748	90. 517	57.472	51.566	1.00 11.91	В	N
ATOM	11786		HIS	748	91.397	56.998	52.430	1.00 12.20	В	Ç
ATOM	11787		HIS	748	91.569	57. 893	53. 384	1.00 9.44	В	N
ATOM ATOM	11788	C	HIS	748	87. 259	58. 310	52.316	1.00 15.00	В	C
ATOM	11789 11790	O N	HIS	748	87. 272	57.097	52. 533	1.00 14.52	В	0
ATOM	11790	CA	GLN	749	86.808	59. 196	53. 200	1.00 14.63	В	N
ATOM	11792	CB	GLN GLN	749 749	86. 283 86. 045	58. 780	54. 496	1.00 15.23	В	C C
ATOM	11793	CG	GLN	749	87.314	59.999	55. 378	1.00 15.87	В	C
ATOM	11794	CD	GLN	749	87.056	60.722	55. 740	1.00 22.62	В	•
ATOM	11795		GLN	749	86. 511	61.956 61.873	56. 564 57. 664	1.00 25.83 1.00 29.51	В	C
ATOM	11796		GLN	749	87. 443	63.116	56.039	1.00 29.51	В	0
ATOM	11797	C	GLN	749	84. 984	57. 999	54. 348	1.00 27.04	B B	N
ATOM	11798	Õ	GLN	749	84. 749	57.015	55. 054	1.00 14.70	В	C 0
ATOM	11799	N	HIS	750	84. 147	58. 440	53. 415	1.00 13.44	В	N N
ATOM	11800	CA	HIS	750	82. 865	57. 808	53. 174	1.00 13.44	В	C
ATOM	11801	CB	HIS	750	82. 021	58.685	52. 247	1.00 12.03	В	C
ATOM	11802	CG	HIS	750	80. 587	58. 272	52. 176	1.00 13.33	В	C
ATOM	11803		HIS	750	79.475	58. 823	52. 713	1.00 12.41	В	Č
ATOM	11804		HIS	750	80.175	57. 128	51.530	1.00 12.98	В	N
ATOM	11805		HIS	750	78. 869	56. 992	51.673	1.00 14.44	В	Č
ATOM	11806		HIS	750	78. 419	58.007	52. 386	1.00 13.43	В	N
ATOM	11807	C	HIS	750	82. 985	56.404	52. 595	1.00 13.84	В	Ċ
ATOM	11808	0	HIS	750	82. 265	55. 499	53. 011	1.00 14.53	B	Ŏ

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					FIC	÷. 4 -	2 4 2			(Continued)
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	11809 11810 11811 11812 11813 11814 11815 11816 11817	CG1 CD1 C O N CA	ILE ILE ILE ILE ILE ILE ILE ILE TYR	751 751 751 751 751 751 751 752 752	83. 885 84. 013 84. 927 86. 326 84. 999 85. 677 84. 546 84. 025 85. 575 86. 137	56. 203 54. 875 54. 838 55. 361 53. 395 53. 240 53. 893 52. 790 54. 284 53. 364	51. 638 51. 077 49. 814 50. 137 49. 287 47. 939 52. 111 52. 241 52. 858 53. 850	1.00 13.03 1.00 12.47 1.00 13.01 1.00 12.55 1.00 12.09 1.00 11.16 1.00 12.65 1.00 12.49 1.00 13.74 1.00 14.04	B B B B B B	N C C C C C C O N C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	11819 11820 11821 11822 11823 11824 11825 11826 11827 11828 11829 11830	CE1 CD2	TYR	752 752 752 752 752 752 752 752 752 753 753	87. 486 88. 628 89. 037 90. 015 89. 235 90. 219 90. 597 91. 536 85. 170 85. 176 84. 323 83. 316	53. 883 53. 468 52. 132 51. 712 54. 383 53. 974 52. 639 52. 223 53. 067 51. 972 54. 040 53. 864	54. 379 53. 472 53. 408 52. 502 52. 608 51. 692 51. 646 50. 739 54. 973 55. 524 55. 295 56. 330	1.00 11.26 1.00 9.86 1.00 10.53 1.00 9.48 1.00 9.66 1.00 8.36 1.00 9.94 1.00 10.79 1.00 13.42 1.00 13.56 1.00 14.48 1.00 14.27	B B B B B B B B	C C C C C C O N C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	11831 11832 11833 11834 11835 11836 11837 11838 11839 11840	CB OG1 CG2 C O N CA CB CG	THR THR THR THR HIS HIS HIS HIS	753 753 753 753 753 754 754 754 754 754	82. 582 83. 519 81. 459 82. 301 81. 958 81. 830 80. 840 80. 424 79. 109 78. 779	55. 187 56. 136 54. 987 52. 849 51. 894 53. 056 52. 163 52. 666 52. 128 51. 362	56. 618 57. 130 57. 629 55. 815 56. 508 54. 589 53. 999 52. 620 52. 162 51. 095	1. 00 13. 68 1. 00 17. 48 1. 00 7. 20 1. 00 16. 15 1. 00 18. 93 1. 00 15. 38 1. 00 16. 06 1. 00 15. 26 1. 00 16. 39 1. 00 15. 75	B B B B B B B	C O C C O N C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	11841 11842 11843 11844 11845 11846 11847 11848 11849	ND1 CE1 NE2 C O N CA CB CG	HIS HIS HIS HIS MET MET MET MET	754 754 754 754 755 755 755 755	77. 936 76. 940 77. 425 81. 349 80. 639 82. 571 83. 158 84. 532 84. 491	52. 353 51. 750 51. 141 50. 731 49. 788 50. 564 49. 234 49. 300 49. 542	52. 850 52. 228 51. 161 53. 886 54. 238 53. 383 53. 250 52. 573 51. 081	1.00 17.30 1.00 15.86 1.00 17.13 1.00 16.28 1.00 17.31 1.00 15.98 1.00 16.05 1.00 15.41 1.00 17.11	B B B B B B	N C N C O N C C C C
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	11850 11851 11852 11853 11854 11855 11856 11857	SD CE C O N CA CB OG	MET MET MET SER SER SER SER	755 755 755 755 756 756 756 756	86. 112 86. 882 83. 309 83. 080 83. 701 83. 854 84. 413 85. 723	49. 308 50. 855 48. 582 47. 390 49. 371 48. 833 49. 903 50. 257	50. 322 50. 742 54. 623 54. 783 55. 614 56. 946 57. 878 57. 477	1.00 18.41 1.00 20.74 1.00 15.38 1.00 13.30 1.00 15.36 1.00 18.52 1.00 18.88 1.00 18.74	B B B B B	S C C O N C C

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					τ	7 T /	2 4	_	243				(Co	ntinued)
					1	. 1 (J. 4	_	43					
ATOM	11858	С	SER	756	82	. 515	48. 28	82	57. 462	1.00	19.14	В	C	
ATOM	11859		SER	756		. 464			57. 975		19.94	В	ő	
ATOM	11860		HIS	757		. 435	49. 04		57. 324		17.68	B	Ň	
ATOM	11861		HIS	757		. 134			57. 770		19. 20	B	Ċ	
ATOM	11862		HIS	757		. 990	49. 48		57. 371		18.83	B	Č	
ATOM	11863		HIS	757		. 983	50. 79		58.095		21.13	B	Č	•
ATOM	11864	CD2		757		. 697	52. 04		57.666		22.10	B	Č	
ATOM	11865	ND1		757		. 230	50. 89		59.447		22.62	В	N	
ATOM	11866	CE1		757		. 096	52. 15		59.820		23.60	В	C	
ATOM	11867	NE2	HIS	757	78	. 772	52.87	76	58.758	1.00	24.81	В	N	
ATOM	11868	C	HIS	757	79	. 866	47. 19	90	57.120	1.00	17.94	В	C	
ATOM	11869		HIS	757	79	.416	46. 28		57.772	1.00	16.58	В	0	
ATOM	11870		PHE	758		. 158	47. 10		55.828		17.93	В	N	
ATOM	11871		PHE	758		. 926	45.88		55.052		18.80	В	C	
ATOM	11872		PHE	758		. 286	46.13		53. 586		15.70	В	C	
ATOM	11873		PHE	758		. 952	44. 99		52.677		10.77	В	C	
ATOM	11874	CD1		758		. 646	44. 79		52. 251	1.00		В	C	
ATOM	11875	CD2		758		. 941	44. 12		52. 254	1.00		В	C	
ATOM	11876	CE1		758		. 334	43. 71		51.409	1.00		В	C	
ATOM ATOM	11877	CE2		758 758		. 638	43. 04		51. 417	1.00		В	C	
ATOM	11878 11879		PHE PHE	758 758		. 340	42.83		50.991	1.00		В	C	
ATOM	11880		rne PHE	758		. 697 . 110	44. 67 43. 63		55. 560		20.68	В	C	
ATOM	11881		ILE	759		. 014	44. 81		55. 851 55. 654		21.00 23.57	B B	0 M	
ATOM	11882		ILE	759 759		. 858	43. 72		56. 117		25.05	В	N C	
ATOM	11883		ILE	759		. 364	44. 12		56.069		25.44	·B	C	
ATOM	11884	CG2		759		. 994	44.04		57. 437		28. 98	В	č	
ATOM	11885	CG1				. 128	43.18		55. 142		26.52	B	č	
ATOM	11886	CD1		759		. 706	43. 26		53. 704		26.84	B	č	
ATOM	11887		ILE	759		. 441	43. 31		57. 529		25. 34	B	Č	
ATOM	11888	0	ILE	759		. 420	42.13		57.866		25.50	В	0	
ATOM	11889		LYS	760	82	. 081	44. 29	19	58.346		26.11	В	N	
ATOM	11890		LYS	760		. 671	44.01	2	59.713	1.00	26.62	В	C	
ATOM	11891		LYS	760		. 444	45.30		60. 487		26.43	В	C	
ATOM	11892		LYS	760		. 178	45. 29		61.792		29.00	В	C	
ATOM	11893		LYS	760		666	45. 27		61.537		28.96	В	C	
ATOM	11894		LYS	760		. 139	46.66		61. 250		30.01	В	C	
ATOM	11895		LYS	760		776	47. 52		62. 420		31.29	В	N	
ATOM	11896		LYS	760		406	43. 17		59. 740		27.08	В	C	
ATOM Atom	11897		LYS	760		312	42. 20		60. 473		28.46	В	0	
ATOM	11898 11899		GLN	761		431	43. 58		58. 940		28.08	В	N	
ATOM	11900		GLN GLN	761 761		170 213	42.86		58. 844		29.69	В	C	
ATOM	11901		GLN	761		072	43. 65 42. 85		57. 942 57. 347		31.26 34.99	В	C	
ATOM	11902		GLN	761		477	42. 00		56. 072		34. 99 37. 85	B B	C	
ATOM	11903		GLN	761		800	42.77		55.062		37. 29	В	C 0	
ATOM	11904	NE2 (761		464	40. 80		56. 112		39.80	B	N	
ATOM	11905		GLN	761		401	41.45		58. 295		30.00	В	Č	
ATOM	11906		GLN	761		791	40. 49		58. 753		31.14	В	Õ	
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					FIC	G. 4-	244			(Oomaniaca)
	44007		OTTO	7.00	70 001	44 000	E7 220	1 00 20 71	В	N
ATOM	11907	N	CYS	762	79. 291	41.333	57. 320	1.00 29.71 1.00 30.30	В	N C
ATOM	11908	CA	CYS	762	79.588	40.035	56. 731 57. 712	1.00 30.30	В	C
ATOM	11909	C	CYS	762	80. 275	39.077	57. 578	1.00 30.21	В	Ö
ATOM	11910	0	CYS	762	80.153		55. 474	1.00 29.01	В	C
ATOM	11911	CB	CYS	762	80. 458		54. 849	1.00 30.01	В	S
ATOM	11912	SG	CYS	762	81.198		58. 698	1.00 30.53	В	N .
ATOM	11913	N	PHE	763	80.986		59.664	1.00 30.33	В	Č
ATOM	11914	CA	PHE	763 763	81.694 83.112		59.885	1.00 31.20	В	č
ATOM	11915	CB CG	PHE	763	84. 052		58. 736	1.00 27.21	В	č
ATOM	11916		PHE PHE	763	83. 663		57.650	1.00 26.19	В	č
ATOM ATOM	11917 11918		PHE	763	85. 348		58. 762	1.00 26.38	B	č
ATOM	11916		PHE	763	84. 552		56.605	1.00 27.91	В	č ·
ATOM	11919		PHE	763	86. 249		57. 727	1.00 27.36	B	č
ATOM	11920	CZ	PHE	763	85. 851		56.643	1.00 27.55	B	Č
ATOM	11922	C	PHE	763	80. 994		61.011	1.00 34.52	B	Č
ATOM	11923	Õ	PHE	763	81.473		61.908	1.00 32.78	В	0
ATOM	11924	Ň	SER	764	79. 862		61.151	1.00 39.49	В	N
ATOM	11925	ĊA	SER	764	79. 099		62.393	1.00 43.60	В	C
ATOM	11926	CB	SER	764	77.860		62.273	1.00 44.56	В	C
ATOM	11927	0G	SER	764	78. 218		61.948	1.00 50.05	В	0
ATOM	11928	C	SER	764	78.668		62.746	1.00 45.96	В	C
ATOM	11929	0	SER	764	77.885		62.028	1.00 45.86	В	0
ATOM	11930	N	LEU	765	79.189	37.404	63.856	1.00 49.22	В	N
ATOM	11931	CA	LEU	765	78.845		64. 317	1.00 52.03	В	C
ATOM	11932	CB	LEU	765	79. 754		65.481	1.00 52.53	В	C
ATOM	11933	CG	LEU	765	81.234		65.115	1.00 52.85	В	Č
ATOM	11934		LEU	765	82.074		66.376	1.00 53.55	В	C
ATOM	11935		LEU	765	81.435	34. 344	64. 214	1.00 52.54	В	C
ATOM	11936	C	LEU	765	77. 383		64. 761	1.00 54.34	В	C
ATOM	11937	0	LEU	765	77.019		65. 743	1.00 53.63	В	0
ATOM	11938	N	PR0	766	76. 523		64.031	1.00 56.38	В	N
ATOM	11939	CD	PRO	766	76.833		62. 831	1.00 56.67	В	C C
ATOM	11940	CA	PRO	766	75.095		64. 356	1.00 57.95	В	
ATOM	11941	CB	PRO	766	74.509		63. 141	1.00 58.24	В	C
ATOM	11942	CG	PRO	766	75.626		62. 728 65. 664	1.00 57.40 1.00 59.30	B B	C C
ATOM	11943	C	PRO	· 766	74. 805 73. 791		65. 711	1.00 55.30	В	0
ATOM	11944	OVT	PRO PRO	766 766	75. 584		66. 627	1.00 59.84	В	0
ATOM TER	11945 11946	UAI	PRO	766	10.009	34, 104	00.041	1.00 05.04	В	U
ATOM	11947	C1	NAG	901	25. 105	38. 477	14. 927	1.00 45.03	E	С
ATOM	11948	C2	NAG	901	26. 266		13. 922	1.00 45.16	Ë	č
ATOM	11949	N2	NAG	901	27. 447		14. 595	1.00 44.20	Ë	N
ATOM	11949	C7	NAG	901	28. 662		14. 153	1.00 43.63	E	Ċ
ATOM	11951	07	NAG	901	29.050		13. 997	1.00 44.60	Ē	ŏ
ATOM	11952	C8	NAG	901	29. 588		13. 838	1.00 43.83	Ē	č
ATOM	11953	C3	NAG	901	25. 942		12. 713	1.00 46.38	Ē	č
ATOM	11954	03	NAG	901	26. 953		11. 728	1.00 49.49	Ē	Ö
ATOM	11955	C4	NAG	901	24. 591		12.124	1.00 47.76	E	С

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						(Continued)
					FIG. 4-245	(Continued)
ATOM	11956	04	NAG	901	24. 256 39. 836 11. 036 1. 00 49	
ATOM	11957	C5	NAG	901	23. 545 39. 104 13. 219 1. 00 49	
ATOM	11958	05	NAG	901	23. 858 38. 173 14. 276 1. 00 47	
ATOM	11959	C6	NAG	901	22.143 38.804 12.731 1.00 50	
ATOM	11960	06	NAG	901	21. 706 39. 781 11. 793 1. 00 53	· · · · · · · · · · · · · · · · · · ·
ATOM ATOM	11961 11962	C1 C2	NAG	902	34. 526 67. 450 4. 248 1. 00 29 33. 682 66. 990 3. 051 1. 00 3	
ATOM	11962	N2	NAG NAG	$\begin{array}{c} 902 \\ 902 \end{array}$	33. 682 66. 990 3. 051 1. 00 33 34. 077 65. 638 2. 692 1. 00 38	
ATOM	11964	C7	NAG	902	33.181 64.660 2.610 1.00 3	
ATOM	11965	07	NAG	902	32. 213 64. 701 1. 852 1. 00 3	
ATOM	11966	C8	NAG	902	33. 392 63. 449 3. 503 1. 00 3'	
ATOM	11967	C3	NAG	902	33. 927 67. 915 1. 848 1. 00 3	
ATOM	11968	03	NAG	902	33.032 67.583 0.794 1.00 34	
ATOM	11969	C4	NAG	902	33. 753 69. 386 2. 248 1. 00 3	
ATOM	11970	04	NAG	902	34.037 70.238 1.144 1.00 30	
ATOM	11971	C5	NAG	902	34.701 69.674 3.412 1.00 30	0.64 E C
ATOM	11972	05	NAG	902	34. 332 68. 844 4. 526 1. 00 30	
ATOM	11973	C6	NAG	902	34.720 71.114 3.892 1.00 30	
ATOM	11974	06	NAG	902	33. 457 71. 512 4. 409 1. 00 34	
ATOM	11975	C1	NAG	903	64. 239 77. 734 14. 341 1. 00 23	
ATOM	11976	C2	NAG	903	63. 984 78. 203 12. 917 1. 00 26	
ATOM	11977	N2	NAG	903	63. 551 77. 080 12. 116 1. 00 28	
ATOM	11978	C7	NAG	903	62.349 77.076 11.551 1.00 24	
ATOM ATOM	11979 11980	07 C8	NAG NAG	903 903	62.121 76.492 10.490 1.00 28	
ATOM	11981	C3	NAG	903	61. 222 77. 800 12. 272 1. 00 23 65. 253 78. 817 12. 325 1. 00 29	
ATOM	11982	03	NAG	903	64. 947 79. 400 11. 066 1. 00 29	
ATOM	11983	C4	NAG	903	65. 814 79. 900 13. 248 1. 00 30	
ATOM	11984	04	NAG	903	67. 092 80. 316 12. 778 1. 00 30	
ATOM	11985	C5	NAG	903	65. 929 79. 389 14. 690 1. 00 30	
ATOM	11986	05	NAG	903	64.669 78.842 15.133 1.00 30	
ATOM	11987	C6	NAG	903	66. 276 80. 502 15. 659 1. 00 32	
ATOM	11988	06	NAG	903	65. 937 80. 144 16. 993 1. 00 38	
ATOM	11989	C1	NAG	904	56.857 73.229 -0.933 1.00 21	1.65 E C
ATOM	11990	C2	NAG	904	58. 289 73. 099 -1. 475 1. 00 21	
ATOM	11991	N2	NAG	904	58.532 71.758 -1.961 1.00 21	
ATOM	11992	C7	NAG	904	58. 567 71. 523 -3. 267 1. 00 20	
ATOM	11993	07	NAG	904	58. 745 72. 412 -4. 104 1. 00 18	
ATOM	11994	C8	NAG	904	58. 371 70. 080 -3. 709 1. 00 20	
ATOM	11995	C3	NAG	904	59. 325 73. 441 -0. 417 1. 00 22	
ATOM	11996	03	NAG	904	60.611 73.413 -1.009 1.00 22	
ATOM ATOM	11997 11998	C4 04	NAG NAG	904 904	59.022 74.832 0.129 1.00 22 59.986 75.217 1.101 1.00 24	
ATOM	11998	C5	NAG	904 904	59. 986 75. 217 1. 101 1. 00 24 57. 634 74. 781 0. 737 1. 00 22	
ATOM	12000	05	NAG	904	56.672 74.506 -0.297 1.00 21	
ATOM	12000	C6	NAG	904	57. 232 76. 083 1. 385 1. 00 24	
ATOM	12002	06	NAG	904	57. 196 77. 133 0. 430 1. 00 31	
ATOM	12003	CI	NAG	905	49.743 85.075 37.084 1.00 31	
ATOM	12004	C2	NAG	905	49.010 86.230 37.756 1.00 33	
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							(Continued)
••	•				FIG. 4-246		
ATOM	12005	N2	NAG	905	47. 823 86. 586 37. 012 1. 0	00 34.30 E	N
ATOM	12006	C7	NAG	905		00 35.18 E	
ATOM	12007	07	NAG	905		00 36.47 E	
ATOM	12008	C8	NAG	905		00 37.15 E	
ATOM	12009	C3	NAG	905		00 33.45 E	
ATOM	12010	03	NAG	905		00 33.93 E	
ATOM	12011	C4	NAG	905		00 35.37 E	
ATOM	12012	04	NAG	905		00 35.45 E	
ATOM	12013	C5	NAG	905		00 34.39 E	
ATOM	12014	05	NAG	905		00 32.56 E	
ATOM	12015	C6	NAG	905		00 36. 29 E	
ATOM	12016	06	NAG	905		00 35.52 E	
ATOM	12017	C1	NAG	906		00 36.45 E	
ATOM	12018	C2	NAG	906		00 37.00 E	
ATOM	12019	N2	NAG	906		00 37.17 E	
ATOM	12020	C7	NAG	906		00 38.41 E	
ATOM	12021	07	NAG	906		00 38.52 E	
ATOM	12022	C8	NAG	906		00 36.25 E	Ċ
ATOM	12023	C3	NAG	906		00 38.66 E	Ċ
ATOM	12024	03	NAG	906		00 39.59 E	Ō
ATOM	12025	C4	NAG	906		0 39.58 E	Č
ATOM	12026	04	NAG	906		0 41.48 E	0
ATOM	12027	C5	NAG	906		0 40. 24 E	C
ATOM	12028	05	NAG	906	129. 556 75. 268 57. 133 1. 0	0 38. 27 E	0
ATOM	12029	C6	NAG	906	131.811 76.032 57.255 1.0	0 41.89 E	С
ATOM	12030	06	NAG	906		0 46.70 E	0
ATOM	12031	C1	NAG	907		0 33.54 E	C
ATOM	12032	C2	NAG	907		0 35.73 E	C
ATOM	12033	N2	NAG	907		0 37.97 E	N
ATOM	12034	C7	NAG	907		0 41.34 E	C
ATOM	12035	07	NAG	907		0 42.96 E	0
ATOM	12036	C8	NAG	907		0 42.60 E	C
ATOM	12037	C3	NAG	907		0 36.63 E	C
ATOM	12038	03	NAG	907		0 38.28 E	0
ATOM	12039	C4	NAG	907		0 35.89 E	С
ATOM	12040	04	NAG	907		0 35.82 E	0
ATOM	12041	C5	NAG	907		0 35.12 E	C
ATOM	12042	05	NAG	907		0 32.61 E	0
ATOM	12043	C6	NAG	907		0 36.17 E	C
ATOM	12044	06	NAG	907		0 38.44 E	0
ATOM	12045	Cl	NAG	908		0 33.83 E	C
ATOM	12046	C2	NAG	908		0 36.51 E	C
ATOM	12047	N2	NAG	908		0 40.33 E	N
ATOM	12048	C7	NAG	908		0 43.03 E	C
ATOM	12049	07	NAG	908		0 45.77 E	0
ATOM ATOM	12050	C8	NAG	908		0 43.86 E	C
ATOM	12051	C3 03	NAG	908		0 37.11 E	C
ATOM	12052 12053		NAG	908		0 37.35 E	0
VIAN	14009	C4	NAG	908	96. 945 63. 975 9. 760 1. 00	O 36.97 E	C

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										(Continued)
					FIG	3. 4 -	247			(00111111111111111111111111111111111111
ATOM	12054	04	NAG	908	96.049	64.165	8.668	1.00 36.08	E	0
ATOM	12055	C5	NAG	908	96.291	63.106	10.841	1.00 35.43	E	C
ATOM	12056	05	NAG	908	97.215	62.906	11.930	1.00 33.34	E	0
ATOM	12057	C6	NAG	908	95.890	61.735	10.341	1.00 36.72	Ε	C
ATOM	12058	06	NAG	908	95.085	61.057	11.296	1.00 38.75	Е	0
ATOM	12059	C1	NAG	909	106.501	80.407	11.987	1.00 55.21	Е	C
ATOM	12060	C2	NAG	909	105.627	81.255	11.048	1.00 55.75	Е	C
ATOM	12061	N2	NAG	909	105.631	82.658	11.427	1.00 55.80	E	N
ATOM	12062	C7	NAG	909	106.748	83. 259	11.828	1.00 56.83	E	C
ATOM	12063	07	NAG	909	107.685	83.526	11.066	1.00 55.16	E	0
ATOM	12064	C8	NAG	909	106.838	83.620	13. 305	1.00 56.25	Ē	C
ATOM	12065	C3	NAG	909	104.195	80.724	11.087	1.0056.36	Е	C
ATOM	12066	03	NAG	909	103.396	81.452	10.166	1.00 58.58	E	0
ATOM	12067	C4	NAG	909	104.176	79.229	10.744	1.00 56.19	E	С
ATOM	12068	04	NAG	909	102.855	78.716	10.862	1.0055.29	E	0
ATOM	12069	C5	NAG	909	105.117	78.478	11.692	1.0056.24	E	С
ATOM	12070	05	NAG	909	106.446	79.028	11.600	1.00 56.65	E	0
ATOM	12071	C6	NAG	909	105. 230	76.996	11. 381	1.00 57.38	E	С
ATOM	12072	06	NAG	909	106.370	76.423	12.010	1.00 55.01	Е	0
ATOM	12073	C1	NAG	910	105. 213	38. 428	20.006	1.00 34.33	E	C
ATOM	12074	C2	NAG	910	106.113	37. 293	19.498	1.00 37.27	E	C
ATOM	12075	N2	NAG	910	107. 447	37. 789	19. 211	1.00 40.05	·E	N
ATOM	12076	C7	NAG	910	108. 495	36.984	19.368	1.00 42.24	E	C
ATOM	12077	07	NAG	910	109.013	36. 771	20. 465	1.00 42.65	E	0 .
ATOM	12078	C8	NAG	910	109.047	36. 295	18. 126	1.00 42.65	E	C
ATOM	12079	C3	NAG	910	105.504	36.650	18. 245	1.00 37.60	E	C
ATOM ATOM	12080	03	NAG	910	106. 296	35. 547	17. 831	1.00 38.44	E	0
ATOM	12081 12082	C4 04	NAG	910	104.084	36. 182	18. 551	1.00 36.63	E	C
ATOM	12082	C5	NAG NAG	910 910	103.489	35.616	17. 388	1.00 37.52	E	0
ATOM	12083	05	NAG	910 910	103. 274 103. 883	37. 387	19.037	1.00 35.81	E	C
ATOM	12085	C6	NAG	910	101.838	37. 930 37. 042	20. 229 19. 385	1.00 34.96 1.00 34.79	E	0
ATOM	12086	06	NAG	910	101. 636	36.089	20. 437	1.00 34.79	E E	C 0
TER	12087	UU	NAG	910	101. (01	30.003	20.401	1.00 34.77	E E	U
ATOM	12088	0	НОН	1	53. 435	80.704	18. 172	1.00 10.60	W	n
ATOM	12089	Ö	HOH	2	57. 473	78. 703	26. 320	1.00 10.00	W.	0 0
ATOM	12090	Ŏ	HOH	3	65. 386	56.077	37. 040	1.00 21.03	W	0
ATOM	12091	Ö	НОН	4	56. 235	76. 520	22. 816	1.00 14.76	W	0
ATOM	12092	Ŏ	НОН	5	58. 127	60.758	28.066	1.00 4.57	Ÿ	0
ATOM	12093	ŏ	НОН	6	40. 099	59.877	48. 410	1.00 16.00	Ÿ	0 .
ATOM	12094	ŏ	НОН	7	29. 796	47. 323	37. 410	1.00 24.76	Ÿ	0
ATOM	12095	Ŏ	НОН	8	38. 634	67. 195	51.371	1.00 22.65	Ÿ	Ő
ATOM	12096	Ö	НОН	9	41.732	52. 103	37.673	1.00 13.34	Ÿ	ŏ
ATOM	12097	Ŏ	НОН	10	79. 275	54. 159	21.409	1.00 15.54	W	0
ATOM	12098	Ŏ	НОН	11	65. 287	66.160	35. 128	1.00 7.29	Ÿ	Ŏ
ATOM	12099	Ö	НОН	12	79. 267	49.364	26.780	1.00 14.00	Ÿ	Ŏ.
ATOM	12100	0	НОН	13	67. 989	56. 792	26.833	1.00 20.21	Ÿ	Ö
ATOM	12101	0	HOH	14.	68. 995	70.138	19.815	1.00 12.98	Ϋ́	Ŏ
MOTA	12102	0	HOH	15	59. 193	63.441	21.787	1.00 5.68	Ÿ	Ö

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					FIG. 4-248		(Continued)
ATOM	12103	0	НОН	16		0 13.21 W	0
ATOM	12103	Ö	HOH	17		0 20.65 W	0
ATOM	12105	ŏ	НОН	18		0 34.74 W	Ö
ATOM	12106	ŏ	НОН	19		0 25.18 W	ŏ
ATOM	12107	Ŏ	НОН	20		0 18.77 W	Ŏ
ATOM	12108	0	НОН	21		0 27.06 W	Ö
ATOM	12109	0	НОН	22		0 29.16 W	0
ATOM	12110	0	HOH	23		0 9.96 W	0
ATOM	12111	0	HOH	24		0 21.66 W	0
ATOM	12112	0	HOH	25	36.753 80.303 31.025 1.0	0 34.33 W	0
ATOM	12113	0	HOH	26		0 10.18 W	0
ATOM	12114	0	HOH	27		0 29.90 W	0
ATOM	12115	0	НОН	28		0 17.51 W	0
ATOM	12116	0	НОН	29		0 34.92 W	0
ATOM	12117	0	HOH	30		0 28.05 W	0
ATOM	12118	0	HOH	31		0 14.46 W	0
ATOM	12119	0	HOH	32		0 22.75 W	0
ATOM	12120	0	НОН	33		0 12.55 W	0
ATOM ATOM	$12121 \\ 12122$	0	HOH HOH	34 25		0 25.33 W	0
ATOM	12123	0	НОН	35 36		0 30.51 W	0
ATOM	12124	0	HOH	37		0 13.22 W 0 21.69 W	0 0
ATOM	12125	ő	НОН	38		0 24.19 W	0
ATOM	12126	ő	НОН	39		0 24.19 W	0
ATOM	12127	Ö	НОН	40		0 22.85 W	0
ATOM	12128	Ŏ	HOH	41		0 12.47 W	0
ATOM	12129	Ŏ	НОН	$4\overline{2}$		0 24.35 W	ő
ATOM	12130	0	HOH	43	* · · · · · · · · · · · · · · · · · · ·	0 32.23 W	ŏ
ATOM	12131	0	HOH	44		0 19.07 W	Ö
ATOM	12132	0.	HOH	45		0 36.05 W	0
ATOM	12133	0	HOH	46		0 20.53 W	0
ATOM	12134	0	HOH	47		0 20.74 W	0
ATOM	12135	0	НОН	48		0 16.65 W	0
ATOM	12136	0	НОН	49		0 18.82 W	0
	12137					0 19.51 W	0
ATOM	12138	0	НОН	51		0 16.49 W	0
ATOM	12139	0	HOH	52 52		0 26.41 W	0
ATOM ATOM	12140 12141	0	НОН	53 E4		0 17.49 W	0
ATOM	12141	0	HOH HOH	54 55		0 24.56 W	0
ATOM	12142	0	НОН	56		0 35.52 W	0
ATOM	12143	0	НОН	50 57		0 10.79 W 0 17.19 W	0
ATOM	12145	Ö	НОН	58		0 17.19 W 0 19.51 W	0
ATOM	12146	0	HOH	59		0 19.51 W	0 0
ATOM	12147	Ö	НОН	60		0 32.17 W	0
ATOM	12148	Ö	НОН	61		0 13. 27 W	0
ATOM	12149	ŏ	НОН	62		0 17. 25 W	0
ATOM	12150	ŏ	НОН	63) 21.54 W	0
ATOM	12151	Ŏ	НОН	64) 22. 27 W	Ö
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										(Continued)
					FI	G. 4	- 249	•		
ATOM ATOM	12152 12153	0	НОН НОН	65 66		84. 458 62. 441		1. 00 38. 65 1. 00 23. 50	W	0
ATOM	12154		HOH	67	56. 514	63. 214	39.402	1.00 20.39	Ÿ	0
ATOM ATOM	12155 12156	0	НОН НОН	68 69		60.456		1.00 37.55	W	0
ATOM	12157	0	НОН	70		51.584 61.634		1.00 22.02 1.00 34.50	W W	0 0
ATOM	12158	ŏ	НОН	71	39. 108			1.00 34.00	W	0
ATOM	12159	0	HOH	72	62.894	85.163	44.724	1.00 38.05	Ÿ	Ö
ATOM	12160	0	HOH	73				1.00 25.50	W	0
ATOM ATOM	12161 12162	0	НОН НОН	74 75		63.405		1.00 31.16	W	0
ATOM	12163	0	HOH	76	76. 481 54. 751	50.940 68.666	55. 523 -3. 038	1.00 8.02 1.00 19.33	W	0 0
ATOM	12164	ŏ	НОН	77		76.851	37. 550	1.00 13.33	W	0
ATOM	12165	0	HOH	78	60.195	69. 793	56.043	1.00 27.75	Ÿ	Ŏ
ATOM	12166	0	НОН	79	68. 721	77. 775	28.423	1.00 14.61	W	0
ATOM ATOM	12167	0	НОН	80	76.538	41.044		1.00 24.17	M	0
ATOM	12168 12169	0	НОН НОН	81 82	27. 643 42. 573	63. 804 57. 621	39. 245 42. 066	1.00 20.70 1.00 19.56	W	0
ATOM	12170	ő	НОН	83	51. 219	56. 139	24. 829	1.00 19.30	W W	0
ATOM	12171	0	HOH	84	64. 281	54. 295	25. 797	1.00 15.83	Ÿ	0
ATOM	12172	0	НОН	85	48.093	54.052	46.307	1.00 38.41	Ÿ	Ö
ATOM ATOM	12173	0	HOH	86	37.006	52. 225	21. 202	1.00 23.83	W	0
ATOM	12174 12175	0	HOH HOH	87 88	44. 149 72. 912	74. 948	5.314	1.00 17.55	₩	0
ATOM	12176	0	НОН	89	52. 329	75. 091 67. 860	28. 633 33. 481	1.00 25.98 1.00 8.31	-W W	0 0
ATOM	12177	Ō	НОН	90	66. 266	74. 773	42. 238	1.00 16.00	W	0
ATOM	12178	0	HOH	91	59. 283	77.076	9.072	1.00 41.29	Ÿ	ŏ
ATOM	12179	0	НОН	92	77. 526	46.454	20. 254	1.00 34.51		0
ATOM ATOM	12180 12181	0	НОН НОН	93 94	59. 751	56.673	29. 191	1.00 24.40	W	0
ATOM	12182	ő	НОН	9 4 95	43. 531 56. 677	63. 248 73. 257	14. 122 -8. 550	1.00 22.64 1.00 18.65	W	0
ATOM	12183	ŏ	НОН	96	64.366	82.016	33. 202	1.00 18.03	W	0 0
ATOM	12184	0	HOH	97	58. 839	62. 776	26. 537	1.00 11.00	Ÿ	Ö
ATOM	12185	0	НОН	98	52. 478	72.152	3.092	1.00 13.58	W	0
ATOM ATOM	12186 12187	0	НОН НОН	99	59.860	59. 389	29. 429	1.00 20.06	W	0
ATOM	12188	0	НОН	100 101	64. 047 44. 369	73. 184 74. 978	44. 557 38. 087	1.00 15.66	W	0
ATOM	12189	Ö	НОН	102	61.861	50. 833	14. 510	1.00 11.11 1.00 31.09	W W	0 0
ATOM	12190	0	HOH	103	40. 708	73.940	22. 137	1.00 13.81	ẅ	0
ATOM	12191	0	HOH	104	51.853	81.601	16.339	1.00 16.73	Ŵ	0
ATOM	12192	0	HOH	105	59.699	55. 348	63. 144	1.00 20.67	W	0
ATOM ATOM	12193 12194	0	НОН НОН	106 107	45. 186 37. 516	81.560	8.416	1.00 13.89	Ä	0
ATOM	12195	Ö	HOH	108	22. 032	59. 183 56. 444	48. 946 27. 934	1. 00 20. 72 1. 00 30. 26	W	0 .
ATOM	12196	Ŏ	НОН	109	65. 773	63. 945	59. 504	1.00 30.20	W	0
ATOM	12197	0	НОН	110	45. 931	73. 798	1.832	1.00 25.56	Ϋ́	0
ATOM	12198	0	HOH	111	29. 602	40.898	24.033	1.00 25.93	Ÿ	0
ATOM ATOM	12199 12200	0	НОН	112	19.080	57. 313	26.663	1.00 20.07	W	0
VION	1 4 4 0 0	0	НОН	113	61.355	50. 296	11.653	1.00 20.49	W	0

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					FI6	G. 4 -	250			Cont	mueu)
						J. T	200				
ATOM	12201	0	НОН	114	41.491	58.601	0.047	1.00 42.91	W	0	
ATOM	12202	0	НОН	115	64. 362	64. 567	16. 259	1.00 24.97	W	ő	
ATOM	12203	Ŏ	НОН	116	43. 928	76. 242	2. 332	1.00 21.69	W	ő	
ATOM	12204	0	НОН	117	80. 703	69. 349	43. 827	1.00 28.64	Ŵ	ő	
ATOM	12205	Ö	НОН	118	81.671	48. 368	20. 456	1.00 15.16	Ÿ	ŏ	
ATOM	12206	ŏ	НОН	119	59.413	71.127	54.004	1.00 22.01	Ÿ	0	
ATOM	12207	ŏ	НОН	120	27. 474	69. 426	47. 288	1.00 26.74	Ÿ	Ő	
ATOM	12208	ŏ	НОН	121	69. 871	60. 279	33. 380	1.00 13.47	Ÿ	Õ	
ATOM	12209	Õ	НОН	122	67.879	38. 425	47. 297	1.00 25.68	Ÿ	Õ	
ATOM	12210	ŏ	НОН	123	41.866	62. 152	36. 306	1.00 27.91	Ÿ	Õ	
ATOM	12211	Õ	НОН	124	82.055	50. 923	20. 718	1.00 23.09	Ÿ	Õ	
ATOM	12212	Ö	НОН	125	38. 821	82.651	33. 998	1.00 14.04	Ÿ	Ö	
ATOM	12213	Õ	НОН	126	64. 420	42. 195	31.710	1.00 28.88	Ϋ́	Õ	
ATOM	12214	Ö	НОН	127	60.713	36. 262	43. 885	1.00 22.95	w	Ŏ	
ATOM	12215	Ŏ	НОН	128	63. 095	38. 041	44. 744	1.00 26.42	Ÿ	Ö	
ATOM	12216	Ŏ	НОН	129	36.718	65. 633	50. 633	1.00 38.12	· W	0	
ATOM	12217	Ŏ	НОН	130	55. 575	80. 086	20. 196	1.00 26.23	w	ő	
ATOM	12218	Ō	НОН	131	41.981	65. 129	15. 577	1.00 23.62	w	ő	
ATOM	12219	Ō	НОН	132	48.067	75. 632	53. 563	1.00 36.38	w	ő	
ATOM	12220	Ö	HOH	133	75.617	59. 792	32.116	1.00 35.58	Ÿ	ŏ	
ATOM	12221	Ō	НОН	134	73. 522	67.486	30. 484	1.00 21.07	Ÿ	ŏ	
ATOM	12222	0	НОН	135	65. 965	81.671	30. 091	1.00 41.74	W	ŏ	
ATOM	12223	0	HOH	136	41.663	53. 300	13. 574	1.00 39.95	Ÿ	ŏ	
ATOM	12224	0	НОН	137	42.885	39.029	29.960	1.00 29.57	Ÿ	ŏ	
ATOM	12225	0	НОН	138	67.606	56.683	24. 253	1.00 37.19	Ÿ	ŏ	
ATOM	12226	0	HOH	139	138. 150	54. 591	37. 133	1.00 19.60	Ÿ	ŏ	
ATOM	12227	0	HOH	140	76.640	48.505	51.547	1.00 22.87	Ÿ	. 0	
ATOM	12228	0	HOH	141	105.346	35.319	45.478	1.00 6.28	Ÿ	ŏ	
ATOM	12229	0	HOH	142	108.946	33.058	43.850	1.00 17.18	Ŷ	Ŏ	
ATOM	12230	0	HOH	143	101.384	50.291	32.321	1.00 12.25	Ÿ	Ö	
ATOM	12231	0	HOH	144	83. 691	56.732	33.886	1.00 18.52	Ÿ	Õ	
ATOM	12232	0	HOH	145	96. 721	59.108	34.335	1.00 14.59	Ÿ	Ō	
ATOM	12233	0	HOH	146	122.411	66.436	57.099	1.00 19.53	Y	Ō	
ATOM	12234	0	HOH	147	107. 303	38.674	48.678	1.00 12.12	W	0	
ATOM	12235	0	HOH	148	102. 207	54.174	15.770	1.00 18.02	W	0	
ATOM	12236	0	HOH	149	104. 534	49. 338	27.730	1.00 13.93	W	0	
ATOM	12237	0	HOH	150	113. 995	67. 497	30.740	1.00 26.00	W	0	
ATOM	12238	0	HOH	151	115. 903	54. 147	45.005	1.00 10.46	W	0	
ATOM	12239	0	HOH	152	114. 104	55.650	9. 401	1.00 27.03	W	0	
ATOM	12240	0	HOH	153	86. 360	55. 414	40.305	1.00 14.32	W	0	
ATOM	12241	0	НОН	154	97. 554	40.670	45. 200	1.00 18.35	Y	0	
ATOM	12242	0	НОН	155	119.087	37. 761	27. 531	1.00 31.02	₩	0	
ATOM	12243	0 ·	НОН	156	87. 809	62.914	36.962	1.00 26.29	W	0 .	
ATOM	12244	0	HOH	157	83. 356	65. 229	44.012	1.00 37.02	Ŋ	0	
ATOM	12245	0	НОН	158	98. 650	46. 435	54. 377	1.00 26.11	W	0	
ATOM	12246	0	HOH	159	99. 982	40.104	43. 504	1.00 11.71	W	0	
ATOM	12247	0	HOH	160	122. 550	42. 243	44.636	1.00 14.84	W	0	
ATOM	12248	0	HOH	161	101.404	56.669	35. 498	1.00 35.54	W	0	
ATOM	12249	0	HOH	162	88. 481	51.896	31.163	1.00 12.64	W	0	

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										(Continued)
					FI	G. 4	- 251			(Continued)
ATOM	12250	0	НОН	163	95. 169			1.00 10.78	W	0
ATOM ATOM	$12251 \\ 12252$	0	НОН НОН	164 165	115. 235			1.00 26.24	W	0
ATOM	12253	0	HOH	166	106. 826 84. 875			1.00 20.62 1.00 36.24	₩	0
ATOM	12254	0	НОН	167	113. 139			1.00 30.24	W	0 0
ATOM	12255	Õ	НОН	168	95. 042		37. 270	1.00 20.30	W	0
ATOM	12256	Ō	НОН	169	76. 879			1.00 23.37	Ψ̈́	0
ATOM	12257	0	HOH	170	114. 148			1.00 18.43	Ÿ	ŏ
ATOM	12258	0	HOH	171	89. 134			1.00 22.93	W	Ŏ
ATOM	12259	0	НОН	172	104. 484		28.628	1.00 23.01	W	0
ATOM	12260	0	НОН	173	97. 990			1.00 35.07	W	0
ATOM	12261	0	HOH	174	108. 093			1.00 23.37	W	0
ATOM ATOM	12262	0	HOH	175	95. 968		51.786	1.00 19.27	W	0
ATOM	12263 12264	0	НОН НОН	176 177	93. 653			1.00 19.54	W	0
ATOM	12265	0	НОН	178	117. 454 96. 322	64. 613 67. 790	44.832	1.00 25.55	W	0
ATOM	12266	0	НОН	179	80. 831	40.760	27. 707 23. 388	1.00 29.36 1.00 28.01	W	0
ATOM	12267	Ŏ	HOH	180	109. 521	38. 188	50. 278	1.00 16.30	W W	0 0
ATOM	12268	0	НОН	181	88. 081	40. 289	29. 465	1.00 7.47	Ÿ	0
ATOM	12269	0	HOH	182	112. 135	42.102	29. 409	1.00 28.14	Ÿ	ŏ
ATOM	12270	0	HOH	183	110.546	33. 279	45.877	1.00 22.55	Ÿ	Ŏ
ATOM	12271	0	НОН	184	101.361	45.858	44.078	1.00 28.83	W	0
ATOM	12272	0	HOH	185	126. 633	38. 023	29. 778	1.00 31.97	W	0
ATOM ATOM	12273 12274	0	HOH	186	122. 283	37. 257	34. 566	1.00 18.77	W	0
ATOM	12275	0 0	НОН НОН	187 188	99. 753	38. 623	40.032	1.00 18.28	W	0
ATOM	12276	0	HOH	189	122. 547 68. 079	56. 954 78. 219	36. 341 33. 025	1.00 20.05	W	0
ATOM	12277	ŏ	НОН	190	134. 519	46. 667	45. 989	1.00 38.49 1.00 34.45	W W	0 0
ATOM	12278	Ŏ	НОН	191	110. 945	39. 354	35. 865	1.00 34.43	W	0
ATOM	12279	0	НОН	192	118. 982	51.843	57. 881	1.00 13.62	Ÿ	0
ATOM.	12280	0	HOH	193	123. 824	35.631	32. 830	1.00 19.19	Ÿ	Ŏ
ATOM	12281	0	HOH	194	100. 524	45.123	38. 393	1.00 26.68	Ÿ	Ö
ATOM	12282	0	HOH	195	122.815	60.696	63.937	1.00 24.15	W	0
ATOM	12283	0	HOH	196	96. 208	59.856	31.652	1.00 12.71	W	0
ATOM ATOM	12284 12285	0 0	НОН НОН	197	80.023	56. 246	54. 587	1.00 10.61	W	0
ATOM	12286	0	нон НОН	198 199	109. 915 96. 990	41.219	37.675	1.00 19.28	W	0
ATOM	12287	Ö	HOH	200	103.494	75. 649 44. 373	27. 926 34. 046	1.00 9.03 1.00 8.20	W	0
ATOM	12288	Ö	НОН	201	97. 045	44. 873	54. 040 53. 124	1.00 8.20 1.00 15.97	W	0 0
ATOM	12289	Ŏ	НОН	202	109.135	58. 341	13. 499	1:00 13.37	Ÿ.	0
ATOM	12290	0	НОН	203	96.465	39. 089	47. 689	1.00 12.68	Ψ̈́	0
ATOM	12291	0	HOH	204	99.669	54. 200	16.885	1.00 13.83	Ÿ	ŏ
ATOM	12292	0	HOH	205	85.350	34.351	33. 261	1.00 15.83	Ÿ	Ö
ATOM	12293	0	НОН	206	106. 252	38. 178	46.273	1.00 17.78	Ÿ	0
ATOM	12294	0	HOH	207	102. 838	63. 592	15.944	1.00 23.96	W	. 0
ATOM	12295	0	НОН	208	114. 173	52. 027	44. 587	1.00 12.16	¥	0
ATOM ATOM	12296 12297	0	НОН НОН	209	114. 209	49. 450	36. 803	1.00 19.70	W	0
ATOM	12297	0	нон НОН	210 211	78. 079	55. 141	59.990	1.00 33.63	W	0
111 (111)	1 4 6 3 0	v	11011	411	95.004	41.032	14. 678	1.00 29.66	₩	0

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ATOM 12399 0 HOH 212 113.170 36.816 43.347 1.00 21.90 W 0 ATOM 12300 0 HOH 213 77.770 71.277 45.572 1.00 31.73 W 0 ATOM 12301 0 HOH 214 128.636 66.746 61.783 1.00 37.87 W 0 ATOM 12302 0 HOH 215 128.566 42.261 18.644 1.00 26.65 W 0 ATOM 12303 0 HOH 216 135.349 43.830 34.280 1.00 24.69 W 0 ATOM 12304 0 HOH 217 85.640 67.686 27.706 1.00 32.33 W 0 ATOM 12305 0 HOH 218 93.669 46.427 45.506 1.00 24.69 W 0 ATOM 12307 0 HOH 219 117.990 67.819 59.317 1.00 20.28 W 0 ATOM 12308 0 HOH 221 117.990 67.819 59.317 1.00 20.28 W 0 ATOM 12307 0 HOH 221 117.228 62.083 29.483 1.00 29.50 W 0 ATOM 12300 0 HOH 221 117.228 62.083 29.483 1.00 29.50 W 0 ATOM 12310 0 HOH 223 105.505 51.938 1.912 1.00 35.19 W 0 ATOM 12310 0 HOH 223 106.835 57.215 14.677 1.00 21.77 W 0 ATOM 12311 0 HOH 224 107.489 60.380 64.395 1.00 24.53 W 0 ATOM 12312 0 HOH 226 116.807 64.679 29.466 1.00 24.83 W 0 ATOM 12313 0 HOH 226 116.807 64.679 29.466 1.00 24.83 W 0 ATOM 12313 0 HOH 228 81.916 67.388 41.878 1.00 24.53 W 0 ATOM 12316 0 HOH 228 81.916 67.898 41.878 1.00 124.19 W 0 ATOM 12317 0 HOH 228 81.916 67.898 41.878 1.00 124.19 W 0 ATOM 12318 0 HOH 228 81.916 67.898 41.878 1.00 124.54 W 0 ATOM 12319 0 HOH 233 106.895 62.265 33.991 1.00 15.40 W 0 ATOM 12312 0 HOH 233 9.799 774 776.73 22.572 1.00 18.00 W 0 ATOM 12313 0 HOH 234 132.069 46.877 32.352 1.00 18.00 W 0 ATOM 12320 0 HOH 234 132.069 46.877 33.339 1.00 29.79 W 0 ATOM 12320 0 HOH 234 132.069 46.877 33.339 1.00 29.97 W 0 ATOM 12320 0 HOH 234 132.069 46.877 33.339 1.00 29.99 W 0 ATOM 12320 0 HOH 234 132.069 46.877 33.339 1.00 29.99 W 0 ATOM 12320 0 HOH 234 132.069 46.877 33.339 1.00 29.99 W 0 ATOM 12330 0 HOH 244 99.571 37.568 48.84 15.71 1.00 12.13 W 0 ATOM 12330 0 HOH 244 99.571 37.568 48.94 1.00 12.13 W 0 ATOM 12330 0 HOH 244 99.571 37.568 48.94 1.00 12.13 W 0 ATOM 12330 0 HOH 244 195.857 52.766 15.499 1.00 29.88 W 0 ATOM 12330 0 HOH 245 110.409 54.086 55.370 1.00 24.76 W 0 ATOM 12330 0 HOH 246 117.307 73.448 16.262 1.00 29.45 W 0 ATOM 12330 0 HOH 247 124.287 57.66 56.87 1.00 19.17 W 0 ATOM 12330 0 HOH 248						FIC	G. 4 -	252			(Continued)
ATOM 12300 0 HOH 213	ATOM	12299	0	НОН	212	113.170	36. 816	43. 347	1.00 21.90	W	0
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ATOM 12339 0 HOH 252 116.022 62.795 46.555 1.00 17.19 W 0 ATOM 12340 0 HOH 253 95.637 65.687 28.739 1.00 22.07 W 0 ATOM 12341 0 HOH 254 89.440 32.347 36.665 1.00 21.89 W 0											
ATOM 12340 0 HOH 253 95.637 65.687 28.739 1.00 22.07 W 0 ATOM 12341 0 HOH 254 89.440 32.347 36.665 1.00 21.89 W 0											
ATOM 12341 0 HOH 254 89.440 32.347 36.665 1.00 21.89 W 0											
AMOST AGGIO O MICHE OFF											
71 DW 17047 V 199 70 70 70 74 74 74 53 NO 1 1 191 7X DX W 7	ATOM	12342	ŏ	НОН	255	86. 628	29. 295	53.611	1.00 21.09	W	0
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<150> US 60/398, 761

<151> 2002-07-29

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Le	u Va	l Th	r II	e Ile	e Th	r Va	l Pr	o Va	l Va	l Lei	ı Lei	ı Ası	n Ly	s Gl	y Thi	•
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ga	t ga	t gc	t ac	a gc	t ga	c ag	t cg	c aaa	a ac	t tac	act	t cta	a ac	t ga	t tac	144
Ası	a Ası	o Al	a Th	r Ala	a Ası	p Sei	r Ar	g Lys	s Thi	r Tyı	Thr	Let	ı Th	r As	p Tyr	•
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Let	ı Lys	s Ası	n Thi	r Tyr	· Arg	g Leu	Lys	Let	і Туі	Ser	Leu	Arg	g Trp	o Il	e Ser	
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Phe	Ile	Leu	Leu	Glu	Tyr	Asn	Tyr	Val	Lys	Gln	Trp	Arg	His	Ser	Tyr	
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ΑI	a Pro) Ala	a Sei	Met	t Leu	ı Ile	Gly	/ Asr	His	з Туі	: Lei	ı Cy:	s Ası	p Va	l Thr	
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Tr	p Ala	a Thi	Glr	ı Glu	ı Arg	; Ile	Ser	Let	Gln	Trp	Lei	ı Arg	g Arg	g Ile	e Gln	
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705		•			710					715					720	
aaa	gcc	ctg	gtc	gat	σt t	gga	σtσ	σat	ttc	മാവ	OT CO	n f or	taa	+ 0 +	o o t	2200

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75

80

70

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Glu	Phe	Gly	His	s Ser	Ile	Asr	ı Asp	Ty1	Ser	· Ile	e Ser	Pro) Asp	Gly	/ Gln
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Phe	lle	Let	ı Leu	ı Glu	Tyr	Asn	Ty:	Val	Lys	Gln	Trp	Arg	g His	Ser	Tyr
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Thr	Ala	Ser	Tyr	Asp	Ile	Tyr	· Asp	Leu	ı Asn	Lys	Arg	Glr	Let	ı Ile	Thr
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Tyr	Ile	Ser	Asn	Glu	Tyr	Lys	Gly	Met	Pro	Gly	Gly	Arg	Asn	Leu	Tyr
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Leu	Asn	Trp	Ala	Thr	Tyr	Leu	Ala	Ser	Thr	Glu	Asn	Ile	Ile	Val	Ala
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Ser	Phe	Asp	Gly	Arg	Gly	Śer	Gly	Tyr	Gln	Gly	Asp	Lys	Ile	Met	His
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Gly	Ser	Gly	Ser	Gly	Val	Phe	Lys	Cys	Gly	Ile	Ala	Val	Ala	Pro	Val
				645					650					655	
Ser	Arg	Trp	Glu	Tyr	Tyr	Asp	Ser	Val	Tyr	Thr	Glu	Arg	Tyr	Met	Gly
			660					665					670		
Leu	Pro	Thr	Pro	Glu	Asp	Asn	Leu	Asp	His	Tyr	Arg	Asn	Ser	Thr	Val
		675					680					685			
Met	Ser	Arg	Ala	Glu	Asn	Phe	Lys	Gln	Val	Glu	Tyr	Leu	Leu	Ile	His
	690					695					700				
Gly	Thr	Ala	Asp	Asp	Asn	Val	His	Phe	Gln	Gln	Ser	Ala	Gln	Ile	Ser
705					710					715					720
Lvs	Ala	Leu	Val	Asp	Val	Glv	Val	Asp	Phe	Gln	Ala	Met	Trp	Tvr	Thr

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725 730 735

Asp Glu Asp His Gly Ile Ala Ser Ser Thr Ala His Gln His Ile Tyr

740 745 750

Thr His Met Ser His Phe Ile Lys Gln Cys Phe Ser Leu Pro

755 760 765

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A. CLASS	IFICATION OF SUBJECT MATTER		
IPC 7	C12N9/48 C07K14/705 G01N23/	20 GO1N33/573	
1	o International Patent Classification (IPC) or to both national classifi	cation and IPC	
	SEARCHED ocumentation searched (classification system followed by classification system followed by classif		
IPC 7	C12N C07K G01N	lion symbols)	
Designation			
Documenta	tion searched other than minimum documentation to the extent that	such documents are included in the flelds search	edi
Electronic d	ata base consulted during the international search (name of data b	ase and, where gradical search terms used)	
1	ternal, WPI Data, PAJ, BIOSIS, EMBA	•	
	ENTS CONSIDERED TO BE RELEVANT		
Category °	Citation of document, with indication, where appropriate, of the re	levant passages	Relevant to claim No.
X	KABASHIMA T ET AL: "DIPEPTIDYL IV FROM XANTHAMONAS MALTOPHILIA: SEQUENCING AND EXPRESSION OF THE GENE AND CHARACTERIZATION OF THE ENZYME"	ENZYME	1,2,6
	JOURNAL OF BIOCHEMISTRY, JAPANES BIOCHEMICAL SOCIETY, TOKYO, JP, vol. 120, no. 6, December 1996 (pages 1111-1117, XP000973151 ISSN: 0021-924X figure 4		
Υ	the whole document	-/	3-5, 14-20
X Funto	er documents are listed in the continuation of box C.	Patent family members are listed in ann	ex.
"A" documer	egories of cited documents : In defining the general state of the art which is not pered to be of particular relevance comment but published on or after the international	'T' later document published after the Internation or priority date and not in conflict with the al- cited to understand the principle or theory invention	oplication but
L documer which is diation	tie it which may throw doubts on priority claim(s) or s cited to establish the publication date of another or other special reason (as specified)	 "X" document of particular relevance; the claimed cannot be considered novel or cannot be convivolve an inventive step when the documen "Y" document of particular relevance; the claimed cannot be considered to involve an inventive 	nsidered to It is taken alone
other m	nt published prior to the international filing date but	document is combined with one or more other ments, such combination being obvious to a in the art.	er such docu-
ialer ina		*& document member of the same patent family Date of mailing of the international search re	mort.
	November 2003	16/12/2003	
Name and ma	alling address of the ISA European Patent Office, P.B. 5818 Patentlaan 2	Authorized officer	
	NL - 2280 HV Riswijk Tel. (+31-70) 340-2040, Tx. 31 651 epo nl, Fax: (+31-70) 340-3016	Bucka, A	

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	ation) DOCUMENTS CONSIDERED TO BE RELEVANT Citation of document, with indication where appropriate of the relevant passages	Rejovent to claim No.
Category °	Citation of document, with indication,where appropriate, of the relevant passages	Relevant to claim No.
Y	ABBOTT CATHERINE A ET AL: "Binding to human dipeptidyl peptidase IV by adenosine deaminase and antibodies that inhibit ligand binding involves overlapping, discontinuous sites on a predicted beta propeller domain" EUROPEAN JOURNAL OF BIOCHEMISTRY, vol. 266, no. 3, December 1999 (1999-12), pages 798-810, XP002261851 ISSN: 0014-2956 the whole document	3-5, 14-20
Y	LAMBEIR A-M ET AL: "A prediction of DPP IV/CD26 domain structure from a physico-chemical investigation of dipeptidyl peptidase IV (CD26) from human seminal plasma" BIOCHIMICA ET BIOPHYSICA ACTA. PROTEIN STRUCTURE AND MOLECULAR ENZYMOLOGY, ELSEVIER, AMSTERDAM, NL, vol. 1340, no. 2, 18 July 1997 (1997-07-18), pages 215-226, XP004281676 ISSN: 0167-4838 the whole document	3-5, 14-20
Y	MEDRANO F J ET AL: "Structure of proline iminopeptidase from Xanthomonas campestris pv. citri: A prototype for the prolyl oligopeptidase family" EMBO (EUROPEAN MOLECULAR BIOLOGY ORGANIZATION) JOURNAL, vol. 17, no. 1, 2 January 1998 (1998-01-02), pages 1-9, XP002261745 ISSN: 0261-4189 the whole document	3-5, 14-20
Α	POLGAR L: "The prolyl oligopeptidase family" CMLS CELLULAR AND MOLECULAR LIFE SCIENCES, BIRKHAUSER VERLAG, BASEL, CH, vol. 59, no. 2, February 2002 (2002-02), pages 349-362, XP002219152 ISSN: 1420-682X the whole document	1-6, 14-20
Α	FULOP V ET AL: "Prolyl oligopeptidase: An unusual beta-propeller domain regulates proteolysis" CELL, CELL PRESS, CAMBRIDGE, NA, US, vol. 94, no. 2, 24 July 1998 (1998-07-24), pages 161-170, XP002221331 ISSN: 0092-8674 the whole document	1-6, 14-20

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tion) DOCUMENTS CONSIDERED TO BE RELEVANT	
Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
AUGUSTYNS K ET AL: "THE UNIQUE PROPERTIES OF DIPEPTIDYL-PEPTIDASE IV (DPP IV/CD26) AND THE THERAPEUTIC POTENTIAL OF DPP IV INHIBITORS" CURRENT MEDICINAL CHEMISTRY, BENTHAM SCIENCE PUBLISHERS BV, BE, vol. 6, no. 4, 1999, pages 311-327, XP000870290 ISSN: 0929-8673 the whole document	1-6, 14-20
ENGEL MICHAEL ET AL: "The crystal structure of dipeptidyl peptidase IV (CD26) reveals its functional regulation and enzymatic mechanism." PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES, vol. 100, no. 9, 29 April 2003 (2003-04-29), pages 5063-5068, XP002261746 April 29, 2003 ISSN: 0027-8424 (ISSN print) the whole document	1-6, 14-20
RASMUSSEN HANNE B ET AL: "Crystal structure of human dipeptidyl peptidase IV/CD26 in complex with a substrate analog." NATURE STRUCTURAL BIOLOGY, vol. 10, no. 1, January 2003 (2003-01), pages 19-25, XP001168693 ISSN: 1072-8368 (ISSN print) the whole document	1-6, 14-20
HIRAMATSU HAJIME ET AL: "The structure and function of human dipeptidyl peptidase IV, possessing a unique eight-bladed beta-propeller fold." BIOCHEMICAL AND BIOPHYSICAL RESEARCH COMMUNICATIONS, vol. 302, no. 4, 21 March 2003 (2003-03-21), pages 849-854, XP002261748 ISSN: 0006-291X the whole document -/	1-6, 14-20
	AUGUSTYNS K ET AL: "THE UNIQUE PROPERTIES OF DIPEPTIDYL-PEPTIDASE IV (DPP IV/CD26) AND THE THERAPEUTIC POTENTIAL OF DPP IV INHIBITORS" CURRENT MEDICINAL CHEMISTRY, BENTHAM SCIENCE PUBLISHERS BV, BE, vol. 6, no. 4, 1999, pages 311-327, XPO00870290 ISSN: 0929-8673 the whole document ENGEL MICHAEL ET AL: "The crystal structure of dipeptidyl peptidase IV (CD26) reveals its functional regulation and enzymatic mechanism." PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES, vol. 100, no. 9, 29 April 2003 (2003-04-29), pages 5063-5068, XP002261746 April 29, 2003 ISSN: 0027-8424 (ISSN print) the whole document RASMUSSEN HANNE B ET AL: "Crystal structure of human dipeptidyl peptidase IV/CD26 in complex with a substrate analog." NATURE STRUCTURAL BIOLOGY, vol. 10, no. 1, January 2003 (2003-01), pages 19-25, XP001168693 ISSN: 1072-8368 (ISSN print) the whole document HIRAMATSU HAJIME ET AL: "The structure and function of human dipeptidyl peptidase IV, possessing a unique eight-bladed beta-propeller fold." BIOCHEMICAL AND BIOPHYSICAL RESEARCH COMMUNICATIONS, vol. 302, no. 4, 21 March 2003 (2003-03-21), pages 849-854, XP002261748 ISSN: 0006-291X the whole document

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		Relevant to claim No.	
	ation) DOCUMENTS CONSIDERED TO BE RELEVANT		
Calegory °	Citation of document, with indication, where appropriate, of the relevant passages	relevant to claim No.	
P,X	OEFNER CHRISTIAN ET AL: "High-resolution structure of human apo dipeptidyl peptidase IV/CD26 and its complex with 1-'('2-'(5-iodopyridin-2-yl)amino!-ethyl!a mino)- acetyl!-2-cyano-(S)-pyrrolidine." ACTA CRYSTALLOGRAPHICA. SECTION D, BIOLOGICAL CRYSTALLOGRAPHY. DENMARK JUL 2003, vol. 59, no. Pt 7, July 2003 (2003-07), pages 1206-1212, XP008024791 ISSN: 0907-4449 the whole document	1-6, 14-20	
			
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International application No. PCT/JP 03/09523

INTERNATIONAL SEARCH REPORT

Box I Observations where certain claims were found unsearchable (Continuation of item 1 of first sheet)				
This International Search Report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:				
1. X Claims Nos.: 7-13 22-24 because they relate to subject matter not required to be searched by this Authority, namely: see FURTHER INFORMATION sheet PCT/ISA/210				
2. X Claims Nos.: 21 because they relate to parts of the International Application that do not comply with the prescribed requirements to such an extent that no meaningful International Search can be carried out, specifically: see FURTHER INFORMATION sheet PCT/ISA/210				
3. Claims Nos.: because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).				
Box II Observations where unity of invention is lacking (Continuation of item 2 of first sheet)				
This International Searching Authority found multiple inventions in this international application, as follows:				
As all required additional search fees were timely paid by the applicant, this International Search Report covers all searchable claims.				
2. As all searchable daims could be searched without effort justifying an additional fee, this Authority did not invite payment of any additional fee.				
3. As only some of the required additional search fees were timely paid by the applicant, this International Search Report covers only those claims for which fees were paid, specifically claims Nos.:				
4. No required additional search fees were timely paid by the applicant. Consequently, this International Search Report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:				
Remark on Protest The additional search fees were accompanied by the applicant's protest. No protest accompanied the payment of additional search fees.				

FURTHER INFORMATION CONTINUED FROM PCT/ISA/ 210

Continuation of Box I.1

Claims Nos.: 7-13, 22-24

Concerning claims 7 to 13 and 22 to 24 applicant's attention is drawn to Rule 39.1(v) PCT.

The subject-matter of claims 7 to 13 and 22 to 24 refers only to the presentation of structural information and is not regarded as patentable invention within the meaning of Rule 39.1(v) PCT. This information is disclosed e. g. as the atomic coordinates listings (or Tables) of a model, their use in a non-technical method, or said information is stored on a diskette/computer.

Thus, the above mentioned claims will not be searched in accordance with Article 17(2)(a)(i) PCT.

Continuation of Box I.2

Claims Nos.: 21

Present claim 21 relates to a product, i. e. an "effector", defined by reference to a desirable characteristic or property, namely as being an effector of dipeptidyl peptidase IV.

The claim covers all products having this characteristic or property, whereas the application provides no support within the meaning of Article 6 PCT and no disclosure within the meaning of Article 5 PCT of any such products. In the present case, the claim so lacks support, and the application so lacks disclosure, that a meaningful search of the claim is impossible.

Independent of the above reasoning, the claim also lacks clarity (Article 6 PCT). An attempt is made to define the product by reference to a result to be achieved. Again, this lack of clarity in the present case is such as to render a meaningful search over the whole of the claimed scope impossible.

Consequently, no search has been carried out under the provisions of Article 17(2)(a)(ii) PCT.

The applicant's attention is drawn to the fact that claims, or parts of claims, relating to inventions in respect of which no international search report has been established need not be the subject of an international preliminary examination (Rule 66.1(e) PCT). The applicant is advised that the EPO policy when acting as an International Preliminary Examining Authority is normally not to carry out a preliminary examination on matter which has not been searched. This is the case irrespective of whether or not the claims are amended following receipt of the search report or during any Chapter II procedure.